AD NUMBER

AD815619

LIMITATION CHANGES

TO:

Approved for public release; distribution is unlimited. Document partially illegible.

FROM:

Distribution authorized to U.S. Gov't. agencies and their contractors; Critical Technology; MAY 1967. Other requests shall be referred to Air Force Weapons Laboratory, WLRT, Kirtland AFB, NM. Document partially illegible. This document contains export-controlled technical data.

AUTHORITY

afwl ltr, 30 nov 1971

NUCLEAR EXPLOSION INTERACTION STUDIES

Volume II

Methods for Analysis of Thermal Phenomena

K. D. Pyatt, Jr., et al.

General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California

Contract AF 29(601)-7035

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. II

May 1967

AIR FORCE WEAPONS LABORATORY
Research and Technology Division
Air Force Systems Command
Kirtland Air Force Base
New Mexico

NUCLEAR EXPLOSION INTERACTION STUDIES

Volume II

Methods for Analysis of Thermal Phenomena

K. D. Pyatt, Jr., et al.

General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California
Contract AF29(601)-7035

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. II

FOREWORD

This report was prepared by General Atomic Division, General Dynamics Corporation, San Diego, California, under Contract AF29(601)-7035. The research was funded by DASA under Program Element 6.16.46.01D, Project 5710, Subtask 07.002, and by ARPA Order 313, Program Element 6.25.03.01.R.

Inclusive dates of research were 22 July 1965 to 21 July 1966. The report was submitted 28 April 1967 by the AFWL Project Officer, Maj George Spillman (WLRT). The contractor's report number is GA-7370.

This final report on Nuclear Explosion Interaction Studies is being published in four volumes. The volume titles are as follows: Volume I, Methods for Analysis of Radiative Transfer; Volume II, Methods for Analysis of Thermal Phenomena; Volume III, Miscellaneous Code Development; and Volume IV, Phenomenology Studies (classified SECRET/RESTRICTED DATA).

The first three volumes are devoted, respectively, to theoretical studies and computer code development in radiative transfer, thermal phenomena, and miscellaneous efforts related to various other aspects of the work. The fourth volume, which is classified, contains the results of applications of these techniques, and of those previously developed, to the study of fireball growth and the interaction of laser radiation with materials.

The NEIS program is long-range, and most of the projects described in this report are in an incomplete state of development. This is due in part to the nature of the existing computer programs themselves, which continue in a state of development as long as they are in use, and in part to the time scale involved in bringing new programs to a state of capability for solving real problems.

General Atomic staff personnel contributing to the research include J.H. Alexander, C.R. Dismukes, R. Durstenfeld, R.S. Engelmore, B.E. Freeman, W.B. Lindley, J.T. Palmer, K.D. Pyatt, L.L. Reed, L.M. Schalit, J.R. Triplett, and numerous others. The cooperation of Col R.H. Pennington, Maj G.R. Spillman, Lt B.S. Chambers, III, Lt N.D. Morgan, Lt R.A. Howerton, Dr. P.V. Avizonis, and Mr. D.W. Lane of the Air Force Weapons Laboratory is gratefully acknowledged.

This report has been reviewed and is approved.

George R. Spillman
GEORGE R. SPILLMAN
Major, USAF
Project Officer

George R. Spillman
for RALPH M. PENNINGTON
Colonel, USAF
Chief, Theoretical Branch

Claude K. Stambaugh
CLAUDE K. STAMBAUGH
Colonel, USAF
Chief, Research Division

ABSTRACT

Various analytic and numerical methods are described for the phenomena which take place when a high-energy-density source interacts with matter. The interaction usually begins with the transient heating of a solid surface for which analytical methods of study have been developed (Section I). The second phase of the interaction process is vaporization. Recent developments in numerical techniques for simulating vaporization are discussed in the context of the two-dimensional interaction code HECTIC (Section II). The third phase normally involves the nonsteady flow of ionized vapor, for which equations of state are required. A general numerical technique (EIONX) for evaluating internal energy and pressure for a given temperature and density has been developed and incorporated in the SPUTTER program (Section III). For computer programs, e.g., HECTIC, which use internal energy and density as the independent variables, numerical methods were developed to invert the equations of state generated by EIONX (Section IV). For relatively low energy-density sources, the vapor may be in a molecular phase for a significant part of the interaction process, thus requiring the development of special techniques for evaluating the molecular dissociation energy as a function of temperature and density. The calculations for one particular material--carbon--are discussed in detail (Section V).

CONTENTS

I. HEATING OF A SLAB BY A TIME-DEPENDENT SOURCE 1
1.1. Introduction 1
1.2. Specification of the Heat Conduction Problem 1
1.3. Example: Heating of a Metallic Slab by a Pulsed Source . . 3
1.4. The Radiation Boundary Condition 7
1.5. Internal Source Deposition 12
1.6. Conclusions 15
References 16

II. VAPORIZATION AND HEAT CONDUCTION IN HECTIC 17
2.1. Introduction 17
2.2. Vaporization 17
2.3. Conduction 23
2.4. Appendix: Glossary and Usage of HECTIC Variables 26
2.5. Appendix: Listing of HECTIC 45

III. EQUATIONS OF STATE FOR IONIZED VAPOR 103
3.1. Introduction 103
3.2. Formulation of the Linear Eionx Routines. 104
3.3. Procedures for Iterative Solution 110
3.4. Program Flow 113
3.5. Communications Blocks 114
3.6. Material Identification 118
3.7. Options 119
3.8. Error Returns 120
3.9. Appendix: Listing of EIONX Routines 122

IV. EQUATION OF STATE INVERSION FROM TEMPERATURE-DENSITY TO SPECIFIC ENERGY-DENSITY BY TABLE LOOK-UP 142
4.1. Introduction 142
4.2. Method 142
4.3. Program GEST 144
4.4. Program EST 146
4.5. Appendix: Mnemonics for GEST and EST 148
4.6. Appendix: Listing of GEST and EST 150

V. EQUATION OF STATE FOR MOLECULAR CARBON 160
5.1. Introduction 160
5.2. Symbols 160
5.3. The System Composition 162
5.4. Thermodynamic Variables 167
5.5. Thermodynamics and Compositions above 7000°K 169
5.6. Low Temperature Results 171
5.7. Coefficients of Fits to Thermodynamic Functions 171
5.8. Interface of CMOL with Other Equation of State Subroutines 173
5.9. Future Improvements 174
5.10. Variable Names Used in CMOL 175
5.11 Appendix: Listing of CMOL 179

DOCUMENTS PRODUCED UNDER CONTRACT AF 29(601)-7035

Alexander, J. H., "Numerical Methods for Solving Two-Dimensional Problems of Radiative Transport," General Atomic Report GAMD-7047, 1966. (Unclassified)

Freeman, B. E., "Polarization Effects on Radiative Diffusion in a Compton Scattering Medium," General Atomic Report GA-6157, 1966, submitted for publication in Astrophys. J.

Palmer, J. T., "A Comparison of Various Difference Schemes for a Simplified One-Dimensional Transport Equation," General Atomic Report GAMD-6955, 1966. (Unclassified)

"Progress Report for Period Ending September 30, 1965" (U), General Atomic Report GACD-6747(9-65), 1965. (SECRET)

"Progress Report for Period Ending December 31, 1965," General Atomic Report GACD-6747(12-65), 1965. (Unclassified)

"Progress Report for Period Ending March 31, 1966," General Atomic Report GACD-6747(3-66), 1966. (Unclassified)

"Progress Report for Period Ending June 30, 1966," General Atomic Report GACD-6747(6-66), 1966. (Unclassified)

Reed, L. L., "Equation of State Inversion from Temperature-Density to Specific Energy - Density by Table Look-Up," General Atomic Report GAMD-7189 (Rev.), 1966. (Unclassified)

Schalit, L. M., and D. R. Yates, "LPLOT Fortran Program," General Atomic Report GAMD-7104, 1966. (Unclassified)

Teichmann, T., "Numerical Integration on a Sphere," General Atomic Report GAMD-6981, 1966. (Unclassified)

Triplett, J. R., "Heating of a Slab by a Time-Dependent Source," General Atomic Report GAMD-6665, 1965. (Unclassified)

SECTION I

HEATING OF A SLAB BY A TIME-DEPENDENT SOURCE

1.1. INTRODUCTION

Analytic solutions of the heat conduction equation may often be used to advantage in the study of interaction phenomena (Ref. 1). Although the analytic treatment must in general neglect both temperature and position dependence of the thermal parameters of the material medium, it is at least not subject to the limitations of accuracy and stability which are encountered in the use of difference equations. The analytic method therefore serves both as a useful guide to the improvement of difference-equation methods and as a convenient check on the validity of particular computational results obtained by use of difference techniques.

1.2. SPECIFICATION OF THE HEAT CONDUCTION PROBLEM

In a typical interaction problem, a semi-infinite region $x > 0$ is occupied by a solid material which is heated by radiation incident upon its surface. The intensity of this source radiation will be denoted by $\dot{E}(t)$ ergs/cm^2/sec, a defined function of time $t > 0$. The present discussion is concerned with the general problem of a source intensity which varies continuously with time. This entire class of problem is definitively treated by Carslaw and Jaeger (Ref. 2).

The absolute temperature of the material medium at position x, time t will be denoted by $T(x,t)$. The material parameters (assumed constant) are given by:

C = Specific heat,

ρ = Density,

k = Thermal conductivity,

$\alpha = \frac{k}{C\rho}$, Thermal diffusivity,

T_B = Absolute temperature of fusion or sublimation,

κ_L = Mass absorption coefficient for source radiation,

$a = \rho\kappa_L$, Volumetric absorption coefficient for source radiation,

R = Surface reflectivity for source radiation,

ϵ = Total emissivity of surface.

In addition, T_0 denotes the initial absolute temperature of the material, T_A denotes the effective blackbody temperature of the external region ($x < 0$), and σ is the Stefan-Boltzmann constant.

The surface fluxes associated with source radiation, thermal radiation, and conduction, are, respectively,

$$\varphi_S(0,t) = (1 - R)\dot{E}(t) \tag{1}$$

$$\varphi_T(0,t) = -\epsilon\sigma \left[T(0,t)^4 - T_A{}^4 \right] \tag{2}$$

$$\varphi_C(0,t) = -k \left.\frac{\partial T}{\partial x}\right|_{x=0} \tag{3}$$

The general boundary condition for the heat conduction problem is

$$-\varphi_T(0,t) + \varphi_C(0,t) = \varphi_S(0,t) \tag{4}$$

Within the solid material, account will be taken of the conductive and source fluxes only, since the measured values of conductivity presumably include a first order contribution from radiative diffusion, and the high order contributions are presumably not more significant than the temperature dependence of the conductivity which is being ignored. If the attenuation of the source flux within the material can be described by a single coefficient a, as in the case of a laser source,

$$\varphi_S(x,t) = (1 - R)\dot{E}(t)\, e^{-ax} \tag{5}$$

The heat conduction equation is then

$$\frac{\partial \varphi_C}{\partial x} + \frac{\partial \varphi_S}{\partial x} + \rho C \frac{\partial T}{\partial t} = 0 \tag{6}$$

or

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t} = -(1 - R) \frac{a}{k} \dot{E}(t)\, e^{-ax} \tag{7}$$

The initial condition

$$T(x, 0) = T_0 , \qquad x > 0 \tag{8}$$

then completes the specification of the problem.

1.3. EXAMPLE: HEATING OF A METALLIC SLAB BY A PULSED SOURCE

In a medium with relatively high conductivity and low transparency for source radiation, the conductive flux will dominate not only the thermal radiative flux at the surface but also the source flux inside the medium; i.e., at times of interest the characteristic depth of the conductive front $\sqrt{\alpha t}$ will be large compared with the characteristic depth of penetration of the source radiation 1/a. The equation to be solved is then the homogeneous heat transfer equation

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t} = 0 , \qquad x > 0,\ t > 0 \tag{9}$$

with boundary condition

$$-k \left.\frac{\partial T}{\partial x}\right|_{x=0} = (1 - R)\, \dot{E}(t) , \qquad t > 0 \tag{10}$$

and initial condition (8).

We note first that, with the aid of Duhamel's Theorem, this problem can be reduced to a simpler problem in which the boundary condition is that the flux be a constant. That is, let

$$T(x,t) = \frac{\partial}{\partial t} \int_0^t \theta(x, t - t_0, t_0)\, dt_0 \tag{11}$$

Then $\theta(x,t,t_0)$ is a solution of the equation

$$\frac{\partial^2 \theta}{\partial x^2} - \frac{1}{\alpha} \frac{\partial \theta}{\partial t} = 0 \tag{12}$$

with

$$-k \left.\frac{\partial \theta}{\partial x}\right|_{x=0} = (1 - R)\, \dot{E}(t_0) \tag{13}$$

and

$$\theta(x, 0, t_0) = T_0 \tag{14}$$

Assume a solution of form

$$\theta = C_0 t^{n/2} f_n\left(\frac{x}{\sqrt{4\alpha t}}\right) + T_0 \tag{15}$$

Then, from Eq. (12), $f_n(z)$ must be a solution of the equation

$$\frac{d^2 f}{dz^2} + 2z \frac{df}{dz} - 2n f = 0 \tag{16}$$

or

$$f_n(z) = i^n \operatorname{erfc}(z) \tag{17}$$

where the functions $i^n \operatorname{erfc}(z)$ satisfy the relations

$$i^n \operatorname{erfc}(z) = \int_z^\infty i^{n-1} \operatorname{erfc}(s)\, ds \tag{18}$$

$$i^{-1} \operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \tag{19}$$

$$2n\, i^n \operatorname{erfc}(z) = i^{n-2} \operatorname{erfc}(z) - 2z i^{n-1} \operatorname{erfc}(z) \tag{20}$$

$$i^n \operatorname{erfc}(0) = \frac{1}{2^n \Gamma\left(\frac{n}{2} + 1\right)} \tag{21}$$

The functions i^0 erfc and i^1 erfc are written as erfc and ierfc, respectively. On imposing the condition (13), one notes first that n = 1, and also that

$$-k \frac{C_0}{\sqrt{4\alpha}} f_1'(0) = (1 - R)\, \dot{E}(t_0) \tag{22}$$

or, using Eqs. (18) and (21) to show that $f_1'(0) = -1$,

$$\theta(x, t, t_0) = \frac{2}{\sqrt{kC\rho}} (1 - R)\, \dot{E}(t_0)\, t^{1/2}\, \text{ierfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) + T_0 \tag{23}$$

From Duhamel's Theorem, Eq. (11), and using also Eqs. (20) and (19),

$$T(x,t) = \frac{2(1-R)}{\sqrt{kC\rho}} \frac{\partial}{\partial t} \int_0^t \dot{E}(t_0)\,(t - t_0)^{1/2}\, \text{ierfc}\left[\frac{x}{\sqrt{4\alpha(t-t_0)}}\right] dt_0 + T_0$$

$$= \frac{1-R}{\sqrt{kC\rho}} \int_0^t \frac{\dot{E}(t_0)}{\sqrt{t - t_0}} \left[\text{ierfc}\left(\frac{x}{\sqrt{4\alpha(t-t_0)}}\right) + \frac{x}{\sqrt{4\alpha(t-t_0)}}\, \text{erfc}\left(\frac{x}{\sqrt{4\alpha(t-t_0)}}\right)\right] dt_0 + T_0$$

$$= \frac{1-R}{\sqrt{\pi kC\rho}} \int_0^t \frac{\dot{E}(t_0)}{\sqrt{t - t_0}}\, e^{-[x^2/4\alpha(t-t_0)]}\, dt_0 + T_0 \tag{24}$$

A pulse shape $\dot{E}(t)$ which has been found useful is

$$\dot{E}(t) = \frac{(m+1)\,E}{2t_1^{\,m+1}}\, t^m, \qquad 0 < t < t_1$$

$$= \frac{(m+1)\,E}{2t_1^{\,m+1}}\, (2t_1 - t)^m, \quad t_1 < t < 2t_1$$

$$= 0 \qquad\qquad t > 2t_1 \tag{25}$$

That is, $\dot{E}$ rises as the m^{th} power of the time to a maximum at time t_1, then decreases in a symmetric manner to zero at time $2t_1$. The width of the pulse at half maximum, Δ, is given by

$$\Delta = 2(1 - 2^{-1/m})\, t_1$$

The constant E is the time integral of $\dot{E}$ over the entire pulse, in ergs/cm^2.

An explicit solution is readily derived for the time interval $0 < t < t_1$, the rising portion of the pulse. In general, for

$$\dot{E}(t) = At^{n/2} \tag{26}$$

where n is an integer not less than -1,

$$T(x,t) = T_0 + A(1-R)(k\rho C)^{-1/2}\Gamma(\tfrac{1}{2}n + 1)(4t)^{\frac{1}{2}n+\frac{1}{2}}\, i^{n+1}\mathrm{erfc}\,\frac{x}{\sqrt{4\alpha t}} \tag{27}$$

The surface temperature is given by

$$T(0,t) = T_0 + A(1 - R)(\pi k\rho C)^{-\frac{1}{2}}\, B(\tfrac{1}{2}n + 1, \tfrac{1}{2})t^{\frac{1}{2}n+\frac{1}{2}} \tag{28}$$

where $B(p,q) = \Gamma(p)\,\Gamma(q)/\Gamma(p + q)$ is the beta function.

Returning to the pulse shape, Eq. (25), the surface temperature may be obtained by substituting Eq. (25) into Eq. (24), setting x = 0, and evaluating the integrals; for m = 4,

$$T(0,t) = T_0 + (\pi k\rho C)^{-\frac{1}{2}}(1 - R)\, At_1^{9/2}\, I(s) \tag{29}$$

where $s = t/t_1$

$$I(s) = \int_0^s \dot{E}(\sigma)\,(s - \sigma)^{-\frac{1}{2}}\, d\sigma$$

$$= \frac{256}{315}\, s^{9/2} - \frac{32}{105}(s - 1)^{3/2}(24s^2 - 48s + 59)\, H(s-1)$$

$$- \frac{256}{315}(s-2)^{9/2}\, H(s-2) \tag{30}$$

$$H(x) = 0, \quad x < 0$$
$$= 1, \quad x \geq 0$$

and

$$A = \frac{(m+1)E}{2t_1^{m+1}} = \frac{5E}{2t_1^5}$$

The dimensionless quantities

$$I(s) = \frac{(\pi k \rho C)^{\frac{1}{2}}}{(1-R)At_1^{9/2}} \left[T(0,t) - T_0 \right] \text{ and } \frac{\dot{E}(s)}{At_1^4}$$

are plotted as functions of s in Fig. 1. The temperature rises as the 9/2 power of the time from t = 0 to t = t_1 and reaches a maximum at approximately 1.10 t_1. This result has been closely reproduced by difference equation solutions to the heat conduction equation.

1.4. THE RADIATION BOUNDARY CONDITION

If the temperature of the surface of the target becomes sufficiently high before sublimation or melting occurs, the blackbody radiation from the surface can no longer be neglected. In the transient regime this radiation condition can become of major importance for the case of refractory nonmetal targets (for a good conductor the conductive flux would still overwhelmingly predominate) when the total energy delivered by the source is near the ablation threshold.

We consider again the homogeneous problem (Eq. (9)) in which the source deposition is assumed to occur only at the surface. The boundary condition is, from Eq. (4),

$$-k \left. \frac{\partial T}{\partial x} \right|_{x=0} + \epsilon\sigma \left[T(0,t)^4 - T_A^4 \right] = (1-R)\dot{E}(t) \qquad (31)$$

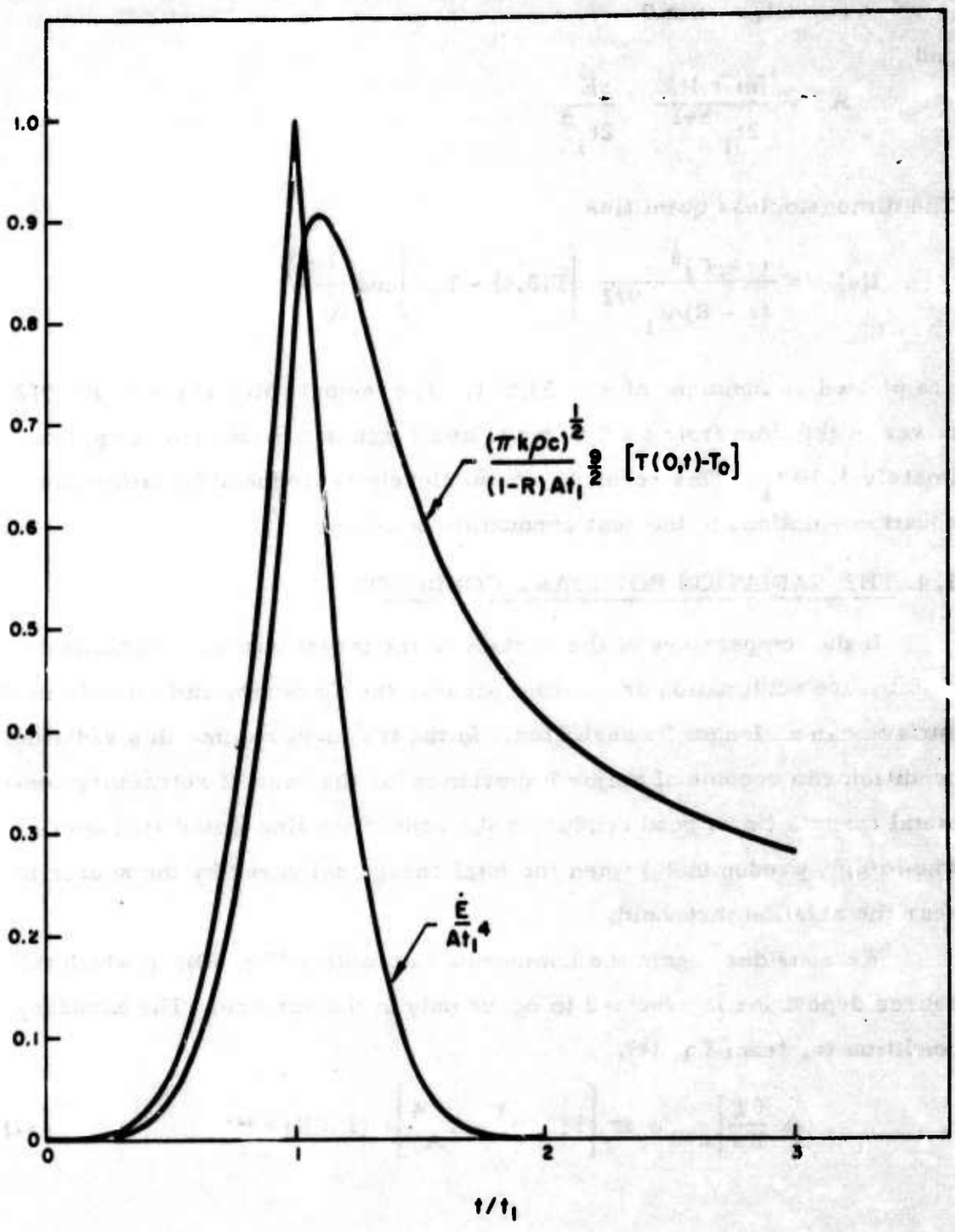


Figure 1. Relative Temperature and Source Intensity versus Time (Dimensionless Plot)

Since this condition is nonlinear in T, some artifice must be employed in order to obtain a solution. Two will be considered:

1. Implicit solution.
2. Linearization.

Linearization is appropriate when the total change of surface temperature during the time of interest is relatively small. However, for refractory materials, which can be heated over a large temperature range, this assumption is not always particularly good. An implicit method which solves the problem with the exact nonlinear boundary condition will therefore be described first. The method is essentially that of Jaeger (Ref. 3).

Assume that $T(0,t)$, $T(0,t)^4$, and $E(t)$ may all be expanded in powers of the variable $z = t^{\frac{1}{2}}$:

$$T(0,t) = T_0 \sum_{n=0}^{\infty} \frac{f_n}{n!} t^{n/2} \equiv T_0 f(z) \tag{32}$$

$$T(0,t)^4 = T_0^4 \sum_{n=0}^{\infty} \frac{g_n}{n!} t^{n/2} \equiv T_0 g(z) \tag{33}$$

$$E(t) = A \sum_{n=0}^{\infty} \frac{h_n}{n!} t^{n/2} \tag{34}$$

The application of the initial condition (8) then provides at once

$$f_0 = 1 \qquad \text{and} \qquad g_0 = 1 \tag{35}$$

The first step in the solution is the derivation of the relations between the g_n and the f_n. Since $g(z) = f(z)^4$,

$$f(z)g'(z) - 4f'(z)g(z) = 0 \tag{36}$$

Differentiating Eq. (36) n times, setting $z = 0$, and noting that $f^{(r)}(0) = f_r$, $g^{(r)}(0) = g_r$, one obtains

$$\sum_{r=0}^{n} \binom{n}{r} (f_r g_{n-r+1} - 4f_{r+1} g_{n-r}) = 0 \tag{37}$$

Equations (35) and (37) may readily be solved explicitly for the g_n:

$$g_0 = 1$$

$$g_1 = 4f_1$$

$$g_2 = 12\, f_1^{\,2} + 4f_2$$

$$\text{etc.} \tag{38}$$

The second step is the solution of the heat conduction equation (9) for the temperature $T_n(x, t)$ when the surface value is a prescribed function of time: $T_n(0, t) = V_n t^{n/2}$, where $V_n = T_0 f_n / n!$. The Laplace transform of Eq. (9) may be written

$$\frac{d^2S}{dx^2} - q^2 S = 0, \qquad x > 0 \tag{39}$$

where

$$S(x) = \int_0^\infty T_n(x, t)\, e^{-pt}\, dt \tag{40}$$

and

$$q^2 = p/\alpha \tag{41}$$

The boundary condition at $x = 0$ is that S shall be the transform of $V_n t^{n/2}$, namely,

$$S(0) = V_n \Gamma(1 + n/2)\, p^{-1-n/2} \tag{42}$$

The solution of Eq. (39) which satisfies this condition and is regular at infinity is

$$S(x) = S(0)\, e^{-qx} \tag{43}$$

The inverse transformation then yields the desired result for the temperature:

$$T_n(x, t) = V_n \Gamma(1 + n/2)\, (4t)^{n/2}\, i^n \operatorname{erfc}\left(\frac{x}{\sqrt{4\alpha t}}\right) \tag{44}$$

Linear superposition of the contributions given by Eq. (44) for each n, as in Eq. (32), then yields the complete solution T(x,t):

$$T(x,t) = T_0 \left[1 + \sum_{n=1}^{\infty} \frac{f_n}{n!} \Gamma(1 + n/2)(4t)^{n/2} \, i^n \mathrm{erfc} \left(\frac{x}{\sqrt{4\alpha t}} \right) \right] \tag{45}$$

It remains to determine the coefficients f_n using the boundary condition (31). The conductive flux at the surface is, from Eqs. (18), (21), and (45),

$$-k \left. \frac{\partial T}{\partial x} \right|_{x=0} = k\alpha^{-1/2} T_0 \sum_{n=1}^{\infty} \frac{\Gamma(1 + n/2)}{n! \, \Gamma(1/2 + n/2)} f_n t^{(n-1)/2}$$

$$= k\alpha^{-1/2} T_0 \sum_{n=0}^{\infty} \frac{\Gamma\left(\frac{3}{2} + \frac{n}{2}\right)}{(n+1)! \, \Gamma(1 + n/2)} f_{n+1} t^{n/2} \tag{46}$$

Substituting Eqs. (46), (33), and (34) into Eq. (31), one finds for n = 0

$$k\alpha^{-1/2} T_0 \frac{\sqrt{\pi}}{2} f_1 + \epsilon\sigma (T_0^4 - T_A^4) = (1 - R) A h_0 \tag{47}$$

and for n > 0

$$k\alpha^{-1/2} T_0 \frac{\Gamma\left(\frac{3}{2} + \frac{n}{2}\right)}{(n+1) \, \Gamma(1 + n/2)} f_{n+1} + \epsilon\sigma T_0^4 g_n = (1 - R) A h_n$$

or for n ≥ 2

$$k\alpha^{-1/2} T_0 \frac{\Gamma\left(1 + \frac{n}{2}\right)}{n\Gamma\left(\frac{1}{2} + \frac{n}{2}\right)} f_n = (1 - R) A h_{n-1} - \epsilon\sigma T_0^4 g_{n-1} \tag{48}$$

The solution, Eq. (45), is thus completely specified. With the coefficients h_n given, one finds first f_1 from Eq. (47), then g_1 from Eq. (38), f_2 from Eq. (48), g_2 from Eq. (38), etc.

An alternative approach to the above is to specify a linearized radiation boundary condition in place of Eq. (31):

$$- \left. \frac{\partial T}{\partial x} \right|_{x=0} + h \left[T(0,t) - T_A \right] = \frac{1 - R}{k} \dot{E}(t) \tag{49}$$

where in some sense

$$h(T - T_A) \sim \frac{\epsilon\sigma}{k} (T^4 - T_A^4) \tag{50}$$

is an adequate approximation for the problem at hand. For problems in which $|T(0,t) - T_A|/T_A \ll 1$ at all times of interest, a good fit is obtained by defining

$$h = h_1 = 4\,\epsilon\sigma T_A^{\,3}/k \tag{51}$$

Equation (51) underestimates the radiative cooling rate for $T(0,t) > T_A$. A second alternative is

$$h = h_2 = \frac{\epsilon\sigma}{k}\,(T_B^{\,4} - T_A^{\,4})/(T_B - T_A) \tag{52}$$

which is correct for $T(0,t) = T_A$ and $T(0,t) = T_B$, but overestimates the cooling rate at all intermediate temperatures. A third alternative, intermediate between h_1 and h_2 in value, is defined by

$$h = h_3 = \frac{\epsilon\sigma}{k}\left[\frac{2}{5}(T_B - T_A)^3 + 2T_A(T_B - T_A)^2 + 4T_A^{\,2}(T_B - T_A) + 4T_A^{\,3}\right] \tag{53}$$

This yields the correct total radiated energy between $T = T_A$ and $T = T_B$, if $T(0,t)$ is a linear function of the time; in this sense it gives an approximately correct mean cooling rate over this interval.

With the initial condition

$$T_0 = T(x,0) = T_A \tag{54}$$

and the boundary condition (49), the general solution is

$$T(x,t) - T_A = \frac{2}{\sqrt{\pi}}(1 - R)\int_0^\infty e^{-hy}\,dy \int_{\frac{x-y}{\sqrt{4\alpha t}}}^\infty \dot{E}\left(t - \frac{(x+y)^2}{4\alpha z^2}\right)e^{-z^2}\,dz \tag{55}$$

(see Ref. 2, p. 74). Other formulas involving the linearized radiation boundary condition are presented in the following section.

1.5. INTERNAL SOURCE DEPOSITION

We consider next the case in which the depth of penetration of the source radiation is not negligible; i.e., at times of interest $\sqrt{\alpha t}$ is not large compared with $1/a$. The source flux must then appear in the differential

equation rather than in the boundary condition. For simplicity, we adopt the initial condition (54) and define $\theta(x,t) = T(x,t) - T_0$. Then the equation to be solved is (7), or in the present notation,

$$\frac{\partial\theta}{\partial t} - \alpha\frac{\partial^2\theta}{\partial x^2} = (1 - R)\frac{a\alpha}{k}\dot{E}(t)\, e^{-ax}, \qquad x > 0 \tag{56}$$

with the linearized radiation boundary condition

$$\frac{\partial\theta}{\partial x} = h\theta\ , \qquad x = 0 \tag{57}$$

and initial condition

$$\theta(x, 0) = 0 \tag{58}$$

The general solution of this problem may be written in the form

$$\theta(x,t) = (1 - R)\frac{a\alpha}{k}\int_0^t dt_0\dot{E}(t_0)\int_0^\infty dx_0\, e^{-ax_0}\, G(x,t\,|\,x_0,t_0) \tag{59}$$

where $G(x,t\,|\,x_0,t_0)$ is the temperature rise at x,t due to a unit source at $x_0, t_0 < t$. Several forms of this Green's function may be written, the choice being one of computational convenience. We introduce first the infinite medium heat conduction kernel

$$U(x,t\,|\,x_0,t_0) = \frac{1}{\pi}\int_0^\infty e^{-\beta^2\alpha(t-t_0)}\cos\beta(x - x_0)\, d\beta \tag{60a}$$

$$= \left[4\pi\alpha(t - t_0)\right]^{1/2}\exp\left[-\frac{(x - x_0)^2}{4\alpha(t - t_0)}\right] \tag{60b}$$

which satisfies the equation

$$\frac{\partial U}{\partial t} - \alpha\frac{\partial^2 U}{\partial x^2} = 0\ , \qquad -\infty < x < \infty, \qquad t > t_0$$

with initial condition

$$U(x, t_0\,|\,x_0,t_0) = \delta(x - x_0)$$

and

$$U \to 0 \text{ as } |x| \to \infty \text{ and as } t \to +\infty$$

This kernel is itself the Green's function for the infinite medium. For our semi-infinite medium, the Green's function may be found by the method of images (Ref. 4):

$$G(x,t\,|\,x_0,t_0) = U(x,t\,|x_0,t_0) + U(x,t\,|-x_0t_0) - 2h\int_{-\infty}^{-x_0} U(x,t\,|y,t_0)\, e^{h(x_0+y)}\, dy \tag{61}$$

$$= \frac{1}{\pi}\int_0^\infty d\beta\; e^{-\beta^2\alpha(t-t_0)}\left[\cos\beta(x-x_0) + \cos\beta(x+x_0) - 2h\int_{x_0}^\infty e^{-h(y-x_0)}\cos\beta(x+y)\,dy\right] \tag{62}$$

$$= \left[4\pi\alpha(t-t_0)\right]^{-1/2}\left|\exp\left[-\frac{(x-x_0)^2}{4\alpha(t-t_0)}\right] + \exp\left[-\frac{(x+x_0)^2}{4\alpha(t-t_0)}\right] - 2he^{hx_0}\int_{x_0}^\infty dy\exp\left[-hy - \frac{(x+y)^2}{4\alpha(t-t_0)}\right]\right| \tag{63}$$

$$= \left[4\pi\alpha(t-t_0)\right]^{-1/2}\left|\exp\left[-\frac{(x-x_0)^2}{4\alpha(t-t_0)}\right] + \exp\left[-\frac{(x+x_0)^2}{4\alpha(t-t_0)}\right] - h\exp\left|h(x+x_0) + h^2\alpha(t-t_0)\right|\operatorname{erfc}\left[\frac{x+x_0+2h\alpha(t-t_0)}{\sqrt{4\alpha(t-t_0)}}\right]\right. \tag{64}$$

Equation (59) has the form of a Laplace convolution, so that if the Laplace transforms of $\theta(t)$, $\dot{E}(t)$, and $G(t-t_0)$ are denoted, respectively, by $\theta(p)$, $\overline{E}(p)$, and $\overline{G}(p)$, then

$$\overline{\theta}(x,p) = (1-R)\frac{a\alpha}{k}\overline{E}(p)\int_0^\infty \overline{G}(p)\, e^{-ax_0}\, dx_0 \tag{65}$$

The transform of the Green's function is

$$\bar{G}(p) = \frac{1}{2\alpha q}\left(e^{-|x-x_0|q} + e^{-(x+x_0)q}\right) - \frac{he^{-(x+x_0)q}}{\alpha q(q+h)} \tag{66}$$

where $q^2 = p/\alpha$ as before. Therefore,

$$\int_0^\infty dx_0\, e^{-ax_0}\bar{G}(p) = \frac{pe^{-ax} - a\alpha q\, e^{-qx}}{p^2 - a^2\alpha p} - \frac{he^{-qx}}{\alpha q\left[q^2 + (h+a)q + ha\right]} \tag{67}$$

and the general result is thus

$$\theta(x,t) = (1-R)\frac{a}{2\pi ik}\int_{c-i\infty}^{c+i\infty} dp\bar{E}(p)e^{pt}\left[-\frac{ae^{-qx}}{q(q^2-a^2)} - \frac{he^{-qx}}{q(q+h)(q+a)}\right] \tag{68}$$

Although this expression involves only a single quadrature, it is not necessarily easier to evaluate than (59), even when $h = 0$. Numerical methods based upon either form are certainly possible and are worth investigating.

1.6. CONCLUSIONS

The analytic approach offers some significant advantages over purely numerical methods of solving difference equations representing the flow of heat. It is not subject to numerical instability difficulties or to truncation error, and simple problems may be solved with far less computational effort than the numerical approach demands. Furthermore, many features of the solution, such as the existence and location of maxima and minima, the leading terms of power series expansions of the solution, and perturbation coefficients which describe the effects of small changes in the parameters of the problem, may be derived directly. Many of these features can be obtained only with considerable difficulty from a numerical treatment.

On the other hand, it must be recognized that the numerical approach is potentially far more powerful and versatile. Temperature-dependent conductivity, the radiation boundary condition, complex time and space dependence of the problem characteristics, and two- or three-dimensional geometry can all be handled within the scope of a practicable calculation

effort. One can, in effect, solve the real problem with which one is presented, rather than some idealized problem which bears an imperfectly known relation to the real problem.

The use of analytic methods within the framework of a basically numerical approach remains to be considered. For example, in a two- or three-dimensional calculation it might be preferable to use a numerical approach based upon the integral formulation (Eq. (59)) rather than the difference equations. Even where the difference equations are entirely adequate, it may require less computer time to evaluate an analytic formula for those cases in which one is available. Purely analytic and purely numerical methods are merely the extremes of a "spectrum" of available approaches; for the majority of problems the most practical techniques probably involve some combination of the two.

REFERENCES

1. Engelmore, R. S., and R. A. Kruger, "Transient Heating and Cooling of a Slab," General Atomic Informal Report GAMD-5538, July 1964
2. Carslaw, H. S., and J. C. Jaeger, Conduction of Heat in Solids, 2nd Ed., Oxford Press, 1959.
3. Jaeger, J. C., Proc. Camb. Phil. Soc. 46 634-41 (1950).
4. Sommerfeld, Arnold, Partial Differential Equations in Physics, Lectures in Theoretical Physics. Vol. VI, Academic Press, New York and London, 1964.

SECTION II

VAPORIZATION AND HEAT CONDUCTION IN HECTIC

2.1. INTRODUCTION

In a two-dimensional geometry the phenomena of vaporization and heat conduction are considerably more complex than in one dimension, and the simplest approaches to the calculations, employing explicit differencing of the partial differential equations involved, are even less feasible than in the one-dimensional case. The approach taken in the effort to develop a two-dimensional Eulerian interaction code has therefore been to concentrate on the analytic description of the physical processes involved in more or less typical applications, rather than on the most general possible solution of the equations. For this reason the approach is essentially one-dimensional.

2.2. VAPORIZATION

The following equations are employed in the description of vaporization at the surface:

Continuity

$$\dot{m} = \rho_o u_a \tag{69}$$

$$\dot{m} = \rho_1 c_1 \tag{70}$$

Equation of motion

$$P_1 + \dot{m} c_1 = P_o + \dot{m} u_a \tag{71}$$

Energy conservation

$$\dot{m}(H_1 + c_1^2/2 - H_o - u_a^2/2) = \varphi_{SV} \tag{72}$$

Vapor equation of state

$$P_1 = (\gamma-1) H'_c \rho_1 \tag{73}$$

Hugoniot pressure in solid[1]

$$P_o = \frac{\alpha^2(1 - \rho_s/\rho_o)}{\rho_s - \beta(1 - \rho_s/\rho_o)^2} \tag{74}$$

These six equations involve seven unknown quantities:

$\dot{m}$ Mass ablation rate,

ρ_o Density on solid side of solid-vapor interface,

ρ_1 Density on vapor side of solid-vapor interface,

c_1 Magnitude of vapor velocity at solid-vapor interface, relative to the interface,

u_a Magnitude of ablation velocity, i.e., velocity of solid relative to the interface,

P_o Pressure on solid side of solid-vapor interface,

P_1 Pressure on vapor side of solid-vapor interface.

The equations also involve seven material parameters, assumed to be known:

H_C Specific internal energy of solid at the vaporization temperature,

H_V Specific internal energy of vaporization,

ρ_s Normal solid density,

H'_C Specific random internal energy of vapor at the interface,

γ Polytropic index of vapor,

α, β Constants in empirical low-pressure state equation for solids:

$P = \alpha u_p + \beta u_p^2$, where u_p is the particle velocity (Ref. 1).

The specific enthalpies of vapor and solid at the interface are defined, respectively, by

$$H_l = H_C + H_V + P_l / \rho_l \tag{75}$$

$$H_o = H_C + P_o / \rho_o \tag{76}$$

Finally, the net energy flux at the interface available for producing vapor, φ_{SV}, is assumed known. In effect,

$$\varphi_{SV} = \dot{E} - \varphi_c \tag{77}$$

where $\dot{E}$ is the total incident flux on the interface and φ_c is the loss due to heat conduction into the interior of the solid. The latter term is treated in detail in Section 2.3. All quantities defined above are non-negative; vector quantities are represented by their magnitudes, since relative orientations are determined by the model assumed. The evaluation of the solid pressure on the Hugoniot replaces the more complete equations of state and motion for the solid, which are not needed for the analysis of many interaction processes. This remains, however, a limitation of the model which may require further developmental effort in the future.

Since the number of equations is one less than the number of unknowns, an additional condition is necessary. The velocity c_l of the vapor at the interface, relative to the interface, must be such that

$$u_a \leq c_l \leq \sqrt{\gamma(\gamma-1)H'_c} \tag{78}$$

That is, it cannot be less than the constant density limit, in which $\rho_1 = \rho_o$, nor greater than the Chapman-Jouguet limit, namely, the local sound speed, for which the entropy is a maximum. If c_1 lies between these limits, the pressure P_1 on the vapor side of the interface is obtainable from the conditions in the external vapor field, for example, by integration back from an exterior boundary condition. In any of these three cases, the additional condition is determined by the hydrodynamic coupling of the vapor at the interface to that beyond the interface. The constant density limit should theoretically be instead a constant pressure limit; i.e., with a more detailed state equation treatment in both vapor and solid, the lower limit of c_1 would appear naturally from the formulation as a condition involving constant pressure across the interface rather than constant density. In the absence of such a more detailed and algebraically involved treatment, the constant density assumption is a reasonable and convenient artifice.

Case 1. Assume first that φ_{SV} is sufficiently small that $c_1^2 = \gamma(\gamma - 1)H'_C$, the Chapman-Jouguet case. Then using Eqs. (69), (70), (71), (73), (75), and (76), Eq. (72) may be written in the form

$$\dot{m}\left[H_V + c_1^2 (1 - u_a/c_1)^2/2 + (\gamma - 1)H'_C (1 - u_a/c_1)\right] = \varphi_{SV} \quad (79)$$

or, since ablation velocity, particularly in this case, must be small compared with the sound speed in the vapor, $u_a/c_1 \ll 1$ and

$$\dot{m} \cong \varphi_{SV} / \left[H_V + c_1^2/2 + (\gamma - 1)H'_C\right] \quad (80)$$

The remaining unknowns are then obtained by solving Eq. (69) for u_a, Eq. (70) for ρ_1, Eq. (73) for P_1, Eq. (71) for P_o, and Eq. (74) for ρ_o. The value of P_1 obtained by this procedure is denoted by P_T, or "P-test".

Case 2. Now assume, in contrast to Case 1, that the relative velocity of the interface and the vapor at the interface is less than the sound speed.

Then the interface remains within the range of influence of the external vapor, and the pressure P_V at the interface may be found as follows. Denote the pressure in the zone adjacent to the interface by P_K, the pressure in the next zone by P_{K+1}, and the widths of the zones by Δ_K, Δ_{K+1}. Then

$$P_V = P_K \quad \text{if} \quad P_K < P_{K+1} \tag{81}$$

$$P_V = P_K + \Delta_K \frac{P_K - P_{K-1}}{\Delta_K + \Delta_{K+1}} \quad \text{if} \quad P_K > P_{K+1} \tag{82}$$

and the true interface pressure is taken to be

$$P_1 = \max (P_T, P_V) \tag{83}$$

If $P_1 = P_T$, i.e., if $P_T > P_V$, the Case 1 calculation already performed is confirmed. Otherwise, it is dropped and the Case 2 calculation is substituted as follows. Equation (79) may be rewritten, using Eqs. (70) and (73) as

$$\frac{1}{2}\left[\frac{(\gamma - 1)H'_C}{P_1} - \frac{1}{\rho_o}\right]^2 \dot{m}^3 + \left[H_V + (\gamma - 1)H'_C \cdot \frac{P_1}{\rho_o}\right] \dot{m} = \varphi_{SV} \tag{84}$$

which is a cubic of the form

$$A\dot{m} + B\dot{m}^3 = \varphi_{SV}$$

Let

$$a = A^2 / \varphi_{SV}^2$$

$$b = \varphi_{SV} / 2B$$

$$S_A = b\left(\sqrt{1 + 4Aa/27B} + 1\right)$$

$$S_B = b\left(\sqrt{1 + 4Aa/27B} - 1\right)$$

The only real root, in physically valid cases, is then

$$\dot{m} = S_A^{1/3} - S_B^{1/3} \tag{85}$$

If $B/Aa = B\varphi_{SV}^2/A^3$ is small, specifically less than 0.01, then S_A and S_B are nearly equal and the form

$$\dot{m} = \frac{\varphi_{SV}}{A}\left(1 - \frac{B\varphi_{SV}^2}{A^3}\right) \tag{86}$$

is used.

The procedure is as follows: Given P_1, evaluate ρ_1 by Eq. (73) and provisionally assign the value ρ_s to ρ_o. Then evaluate $\dot{m}$ by Eq. (85) or (86), u_a by Eq. (69), c_1 by Eq. (70), and P_o by Eq. (71). If $\rho_1 \leq \rho_o$ or equivalently $P_1 \leq (\gamma - 1)H'_C \rho_o$, the calculation is then complete. If however, $P_1 > (\gamma - 1)H'_C \rho_o$, first try re-evaluating ρ_o from Eq. (74) to determine if the solid has been shocked to a sufficiently high density to pass the test. If this is insufficient, the Case 2 calculation is dropped and the Case 3 calculation is substituted.

Case 3. This is the constant density case; the solution is given by setting $P_o = P_1$, solving Eq. (74) for ρ_o, and setting $\rho_1 = \rho_o$. Since by Eq. (71) $c_1 = u_a$, Eq. (72) reduces to

$$\dot{m} = \frac{\varphi_{SV}}{H_V} \tag{87}$$

which is essentially equivalent to

$$\dot{m} = \frac{\dot{E}}{H_V + H_C} \tag{88}$$

since conductive steady state is quickly achieved under these conditions. Finally, u_a is determined by Eq. (69).

The HECTIC code at the present time employs a still simpler procedure in which ρ_o is identified with ρ_s under all conditions so that Eq. (74) is not used at all. The procedure described above merely indicates refinements which can be readily made without modifying the vapor state equation or introducing a complete solid state equation into the formulation.

2.3. CONDUCTION

The basic equation for the description of heat flow in the solid is

$$\rho_o C_V \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial s^2} + q(s,t) \tag{89}$$

where $q(s,t)$ represents the net source of heat at a fixed position s. It is convenient to transform this equation to a moving coordinate x such that

$$s = x + \frac{\dot{m}}{\rho_o} t \tag{90}$$

i.e., x represents the depth in the solid relative to the moving solid-vapor interface. The transformed equation is then

$$\rho_o C_V \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial x^2} + \dot{m} C_V \frac{\partial \theta}{\partial x} + q , \qquad x \geq 0 \tag{91}$$

The additional term $\dot{m} C_V \, \partial\theta/\partial x$, which is negative, represents an effective reduction of the heating rate at a point x as this point moves down the temperature gradient. The term q is defined by

$$q = \dot{Q}(x,t) - \varphi_{SV} \, \delta(x) \tag{92}$$

where $\dot{Q} = -(\partial \dot{E}/\partial x)$ is the local heating rate due to the external source and the second term accounts for the energy removal by vaporization at the interface, which is to be computed.

The physical model is that of an initially cold solid, which is heated by the incident flux until the surface temperature reaches H_C/C_V, at which time vaporization begins. On the assumption that at a time t the depth of

the conductive front $\sqrt{\alpha t}$ (where $\alpha = k/C_V \rho_o$ is the thermal diffusivity) is large compared with the characteristic depth of the solid in which the source $\dot{E}$ is deposited, the temperature is given by the general formula (Ref. 2) (cf. Eq. (24) in Section 1):

$$\theta(x,t) = (\pi k C_V \rho_o)^{-1/2} \int_o^t \frac{\dot{E}(0,t')}{\sqrt{t-t'}} e^{-x^2/4\alpha(t-t')}\, dt' \qquad (93)$$

If, as is usually the case, the deposition depth can be neglected by the time the surface begins to vaporize, then this time t_c can be determined from Eq. (93):

$$\theta(0,t_c) = H_C/C_V = (\pi k C_V \rho_o)^{-1/2} \int_o^{t_c} \frac{\dot{E}(0,t')}{\sqrt{t_c - t'}}\, dt' \qquad (94)$$

At time t_c the temperature distribution near the surface, given by Eq. (93), may be expanded in powers of x:

$$\theta(x,t_c) = \frac{H_C}{C_V}\left[1 - \frac{C_V \dot{E}(0,t_c)}{k H_C}\, x + 0(x^2)\right] \qquad (95)$$

which implies that the conductive flux at the surface

$$\varphi_c = -k \left.\frac{\partial\theta}{\partial x}\right|_0 \qquad (96)$$

is equal to the source flux $\dot{E}(0,t_c)$. This is equivalent to stating that there is (for $t \leq t_c$) no surface singularity to make the energy flux discontinuous. It is also the case that the distribution of temperature defined by Eq. (93) is roughly exponential in x, and that this general shape holds at later times as well. The approximation

$$\theta(x,t) = \frac{H_C}{C_V} e^{-x/z(t)}, \qquad t \geq t_c,\ x \geq 0 \qquad (97)$$

where, according to Eq. (95),

$$z(t_c) = \frac{kH_C}{C_V \dot{E}(0, t_c)} \tag{98}$$

is therefore not unreasonable, particularly in view of the fact that the detailed spatial distribution of temperature in the solid is not of interest.

The specification of the function z(t) may be made by substituting Eq. (97) into the two first-derivative terms of Eq. (91) and integrating over x from -0 to ∞;

$$\rho_o H_C \frac{dz}{dt} = [\varphi_c(\infty) - \varphi_c(-0)] - \dot{m}H_C + \dot{E} - \varphi_{SV} \tag{99}$$

Since the conductive flux vanishes at infinity, and also at -0, which is beyond the interface, the result is

$$\frac{dz}{dt} = \frac{1}{\rho_o H_C} [\dot{E}(0, t) - \dot{m}H] \tag{100}$$

where H, the total specific energy for heating and vaporization, is given by

$$\dot{m}H = \varphi_{SV} + \dot{m}H_C \cong \dot{m}[H_C + H_V + c_1^2/2 + (\gamma - 1)H'_C] \tag{101}$$

(which follows from Eq. (79) with $u_a/c_1 \ll 1$). The differential equation (100), with initial condition (98) therefore describes the advance of the conductive front in a straightforward manner, and provides a simple approximation to the true solution of the heat conduction equation. The explicit difference representation of Eq. (100) is solved at the conclusion of each cycle, following the vaporization procedure described above. The conductive flux, Eq. (96), is then calculated as

$$\varphi_c = \frac{kH_C}{C_V z(t)} \tag{102}$$

and the quantity φ_{SV}, defined by Eq. (77), is then updated.

2.4. APPENDIX: GLOSSARY AND USAGE OF HECTIC VARIABLES

Tables I and II list those variable names in common storage which are currently in use, and their relative locations, definitions, and defined values, if any. All units are in the cgs system, except for temperature, which has units of electron volts. A "specific" quantity always means "per unit mass," i.e., "per gram." Variable names followed by an asterisk are input quantities.

Various quantities associated with boiling are stored in the SOLID array. For each value of the radial cell index I, there may be up to 20 such quantities. Since the total array size is 400, a maximum of 20 "boiling" cells is permitted. With the assumption that J = 20 (I - 1) +1, the quantities SOLID (J+N) are defined in Table II for various values of N.

Table III is a cross-referencing of all the variable names and the subroutines which use common storage. As "X" in the table indicates that the variable listed on that row is used at least once by the subroutine listed in that column.

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC

Variable name	Loc	Definition
PRØB	1	Problem identification number
CYCLE	2	Cycle number
DT	3	Time step Δt^n
PRINTS*	4	Cycle frequency for short prints
PRINTL*	5	Cycle frequency for long prints
DUMPT 7*	6	Cycle frequency for tape dumps
CSTØP*	7	Maximum allowed cycle number
PI	8	3.1415927
SCYCLE *	10	Start cycle number; if positive will search dump tape; if zero will generate mesh and start from time zero
SPRØB *	11	Problem identification number; used to check against PRØB read from restart dump tape
ETH	13	Total energy in system
FFA *	14	Maximum allowed increase in Δt per cycle (2.)
FFB *	15	Minimum allowed Δt (10^{-10} sec)
XMAX	18	Largest value of the radial coordinate
DNN	23	Used in EDIT to calculate the energy check number ECK
DMIN *	24	Maximum allowed value of ECK
DTNA	26	Time step on previous cycle Δt^{n-1}
NC	30	Integer value of cycle number
NPC	31	Number of cycles between short prints
IMAX	33	Number of zones in the radial direction
IMAXA	34	IMAX + 1
JMAX	35	Number of zones in the axial direction

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
JMAXA	36	JMAX +1
KMAX	37	(IMAX) (JMAX) +1
KMAXA	38	KMAX +1
I1	47	Active grid counter in the radial direction +2
I2	48	Active grid counter in the axial direction +2
N1 *	51	Input to SETUP; number of Δx_1's or Δy_1's
N2 *	52	Input to SETUP; number of Δx_2's or Δy_2's
N3 *	53	Input to SETUP; number of Δx_3's or Δy_3's
N4 *	54	Input to SETUP; number of Δx_4's or Δy_4's
N7	57	Dump tape number
NRM	62	Maximum permitted number of radiation cycles per hydrocycle; currently inoperative (bypassed when SN<O)
TRAD	63	Radiation time step (currently not used)
SN *	65	Switch in PH1 to cause backward integration in time to correct the integration of internal energy (this occurs when SN = O and UT > O) (-1.)
ECK	76	Energy check criterion. At the short-print cycle frequency, the relative error between ETH and the sum over cells of internal and kinetic energy is formed and stored in WSA. The difference between WSA and its value at the last short print cycle, divided by NPC, is the quantity ECK

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
T	84	Total time to cycle N
S1	90	Error flag. Its value indicates the subroutine in which the error occurred
HVB *	100	Heat of vaporization (specific)
HCB *	101	Heat required to bring solid to boiling point (specific)
SVS *	103	Specific volume of solid
ATØM *	104	Atomic weight of material
CV *	105	Specific heat of solid
GV *	106	γ of vapor at vaporization temperature
ANN *	110	Exponent for laser pulse function
EZERØ *	111	Total laser pulse energy per unit area
PW *	112	Pulse width at half-maximum for laser source
CAPS *	113	Laser absorption coefficient in solid material
HNU *	114	Laser photon energy (ev)
COE *	115	Coefficient used in calculation of laser absorption coeff. at temperature below 2 ev.
SCR	116	Incident laser flux; derivative of the laser pulse function
ISR *	117	Index of largest radial zone irradiated by source
SCDR	118	Duration of source
AHN	119	8.62×10^{10} (ATØM * HNU)^2
DTH	120	Shortest cell transit time in the mesh, i. e. the minimum value of $\Delta x/u$ or $\Delta y/v$

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
IH	121	I value of cell determining DTH
JH	122	J value of cell determining DTH
DTC	123	Δt determined by Courant stability condition
IC	124	I value of cell determining DTC
JC	125	J value of cell determining DTC
RFT *	126	Reflectivity of target surface to laser radiation
CDUT *	127	Conductivity of target material
HCP *	128	Energy of gas at zero temperature $-(H_c+H_v)$
HH	129	Enthalpy of gas at the boiling point
CØ	130	Sound speed in gas at the boiling point
J5*	135	J value of vapor zones adjacent to the solid-vapor interface
SVMAX *	138	Maximum specific volume allowed at free surface; no mass flows to the outer cells if the specific volume exceeds SVMAX (10^{14})
FRCDTC*	139	Fraction of DTC used to determine Δt (0.5)
VAPE	140	Total internal and kinetic energy in vapor
RADE	141	Total reflected source energy; this energy is lost from the system
CNDE	142	Total energy conducted to interior of target
SCRE	143	Total incident energy from source
IV	144	I value of cell which determined DTVF
JV	145	J value of cell which determined DTVF

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
IU	146	I value of cell which determined DTUF
JU	147	J value of cell which determined DTUF
DTVF	148	Axial free surface velocity time control
DTUF	149	Radial free surface velocity time control
EI1 *	150	Constant used to compute laser absorption coefficient
X(I)	152	Radial coordinate, measured to outer boundary of cell
FLEFT (I)	205	Radial momentum flux across left boundary in PH2
UL(I)	205	Weighted velocity on left boundary of cell in PH1
YAMC (I)	305	Axial momentum flux across left boundary in PH2
GAMC (I)	405	Mass flux across left boundary in PH2
PL (I)	405	Pressure on left side of cell in PH1
PR (I)	405	Temporary storage in INPUT and EDIT
SIGC (I)	505	Total specific energy flux across left boundary in PH2
THETA (I)	605	Cell temperature
Y (I)	1806	Axial coordinate, measured to upper boundary of cell
AIX (I)	1907	Specific internal energy of cell
AMX (I)	3109	Mass in cell
DX (I)	4315	Radial cell width
DY (I)	4367	Axial cell width
P (I)	4472	Cell pressure
PIDTS	5674	Working storage in PH1 and PH2

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
PRR	5676	Average of cell pressure and pressure in zone on the right
RC	5933	X coordinate of cell center
RHØ (I)	5935	Cell density
RR	7136	X coordinate of center of cell on the right
SIG	7137	Working storage in CDT
TAU (I)	7190	Area of ring I: $\pi(x_{i+1}^2 - x_i^2)$
TAUDTS	7242	TAU (I) * DT in PH1
U (I)	7244	X-component of cell velocity
URR	8445	Weighted average of cell velocity U(I) and cell on right
UT	8446	Recycle variable in PH1 (-1, 0, or +1)
UU	8447	New Δt for recycling in PH1
UVMAX	8450	(Max. U or V)/(Min. Δx or Δy) in CDT
V (I)	8451	Y- component of cell velocity
VABOVE	9651	Velocity V in cell above
VBLØ	9652	Velocity V in cell below
VEL	9653	Tag in PH1 to note pass number
W2 (I)	9660	Laser radiation flux arriving at solid-vapor interface
WS	9761	Working storage
WSA	9762	Working storage
WSB	9763	Working storage
I	9774	Radial index
IWSA *	9779	Generator input: last card if = +1
IWSB *	9780	Generator input: x, Δx data if 0; y, Δy data if 1

Table I

STORAGE LOCATIONS AND DEFINITIONS OF VARIABLES USED IN HECTIC (Continued)

Variable name	Loc	Definition
J	9832	Axial index
K	9836	Cell index, a composite of I and J
KP	9838	K + IMAX
L	9841	Running index in certain loops
M	9842	Running index in certain loops
MZ	9848	Number of words in the Z array (150)
N	9849	Temporary storage for zone index
NK	9850	Working storage
NK1	9852	Working storage
NR	9854	Number of radiation cycles per hydro-cycle (currently inoperative)
SØLID (I)	9905	See Table II
TEMP (I)	10305	Temporary storage
FIØUT (I)	10317	Source energy flux leaving cell
CAP (I)	11517	Used for both K_{Laser} and $\bar{Z}$
KFIT (I)	12717	Array for packed flags
ISEND, ISL	13917	Indicator for last cycle
IGØTØ	13918	Indicator in EDIT for type of print out
HEAD (I)	13919	Storage for problem identification heading

Table II

LAYOUT OF VARIABLES STORED IN SOLID

N	Definition
1	z, an effective conduction length for calculating the conductive heat loss at the surface
2	φ_{SV}, the net heating rate at the surface
3	E_C, the total heat loss into the interior
4	φ_s, the incident laser energy delivered per unit area up to time t
5	Not used
6	$\dot{m}$, the mass ablation rate
7	m, the mass ablated per unit area
8	$\varphi_{s,surf}$, the incident laser energy delivered to the surface per unit area up to time t
9	Not used
10	P_v, the vapor pressure at the interface
11	P_{test} (see discussion of boiling)
12	P_o, the pressure on the solid side of the interface
13	I, the impulse per unit area, found by integrating P_o
14	Mass ablated on this cycle
15	v_1, the velocity of injection of vaporized matter
16	Not used
17	Not used
18	Not used
19	Not used
20	Not used

Table III

CROSS REFERENCE OF HECTIC VARIABLES

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
A, AREA		4309														
AHN		119											x			x
AID		1906														
AIX	1200	1907		x	x	x	x		x	x			x			
ALCØ		109														
AM		3107											x			
AMD		3108														
AMDM		21														
AMK	15	220														
AMX	1200	3109		x	x	x	x		x	x			x			
AMXM		22														
ANN		110					x						x			
ATOM		104											x			x
BBOUND		74														
BETA		108														
BIG		4310														
BOUNCE		4311														
CABLN		82														
CAP	1200	11517		x	x		x						x			
CAPS		113														x
CB		102											x			
CDUT		127						x					x			
CNDE		142			x			x					x			
CØ		130						x		x			x			
CØE		115											x			x
CSTØP		7			x											
CV		105						x					x			
CVIS		27														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
CYCLE		2		x	x	x							x	x		
DDVK		4313														
DDXN		4312														
DKE		605														
DMIN		24			x											
DNN		23			x											
DT		3			x	x	x	x	x	x			x			
DTC		123			x	x							x			
DTH		120			x	x							x			
DTNA		26				x			x				x			
DTRAD		70														
DUMPT 7		6			x											
DVK		4314														
DX	52	4315		x	x	x			x	x			x			
DXN		66														
DY	100	4367		x	x	x	x		x	x			x			
E		4467														
ECK		76			x											
ETH		13			x		x		x	x			x			
EZERØ		111					x						x			
FD		4468														
FEF		25														
FFA		14				x										
FFB		15				x										
FIØOUT	1200	10317		x	x		x			x			x			
FLEFT	200	205								x						
FS		4469														
FX		4470														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	CS	ESK
G	50	9855														
GAM, SCYCLE		10		x												
GAMC	100	405								x						
GAMD, SPRØB		11		x												
GAMX		12														
GMADR		88														
GMAX		85														
GMAXR		89														
GV		106						x		x			x			
HCB		101						x		x			x		x	
HCP		128						x		x			x		x	
HEAD	12	13919		x										x		
HH		129						x					x			
HNU		114											x			x
HVB		100						x		x			x		x	
I		9774		x	x	x	x	x		x	x	x	x	x		
IC		124			x	x										
IH		121			x	x										
II		9775														
IMAX		33		x	x	x	x	x	x	x	x		x			
IMAXA		34											x			
IN		9776														
IR		9777														
ISL, ISEND		13917	x	x	x					x						
ISR		117			x		x	x	x	x			x			
IWS		9778														
IWSA		9779											x			
IWSB		9780											x			

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
IWSC		9781														
IW1	50	9782														
IXMAX		[illegible]														
IZ	150	1			x	x							x			
I1		47			x					x	x					
I2		48			x						x	x				
I3		49														
I4		50														
J		9832		x	x	x	x	x	x	x	x		x			
JC		125			x	x										
JH		122			x	x										
JMAX		35		x	x	x				x		x				
JMAXA		36			x								x			
JN		9833														
JP		9834														
JR		9835														
J1		131														
J2		132														
J3		133														
J4		134														
J5		135			x		x	x		x		x	x			
J6		136														
K		9836			x	x	x	x	x	x			x			
KDT		41														
KFIT	1200	12717		x	x	x	x	x	x	x			x			
KMAX		37			x								x			
KMAXA		38		x	x								x			
KN		9837														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRING	ES	ESK
KP		9838								x						
KR		9839														
KRM		9840														
L		9841		x	x			x		x			x			
LP, IGØTØ		13918			x					x						
M		9842			x								x			
MA		9843														
MB		9844														
MC		9845														
MD		9846														
ME		9847														
MZ		9848		x	x											
N		9849					x		x				x			
NC		30			x	x	x									
ND		40														
NIMAX		45														
NJMAX		46														
NK		9850			x								x			
NKMAX		9851														
NK1		9852			x											
NMAX		39														
NØ		9853														
NØD		943														
NØPR		44														
NPC		31			x	x										
NPR		28														
NPRI		29														
NR		9854		x					x							

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	D"LOW	SETUP	SPRINT	ES	ESK
NRC		32														
NRM		62							x							
N1		51											x			
N1O		60														
N11		61														
N2		52														
N3		53											x			
N4		54											x			
N5		55											x			
N6		56														
N7, NTAPE		57		x	x											
N8		58														
N9		59														
ØUT		4471														
P	1200	4472		x	x	x		x	x	x			x			
PABØVE		5672							x							
PBLØ		5673							x							
PIDTS		5674							x	x						
PIDY		8					x		x	x			x			
PK	15	235														
PL	100	405							x							
PPABOV		5675														
PR	100	405			x											
PRINTL		5			x											
PRINTS		4			x											
PRØB		1		x	x								x			
PRR		5676							x							
PUL	225	5677														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
PW		112											x			
QDT		5932														
QK	15	250														
Q000FL		7138														
RADE		141			x								x			
RADEB		69														
RADER		67														
RADET		68														
RC		5933							x							
REZ		5934														
REZFCT		71														
RFT		126											x			
RHØ	1200	5935		x	x	x	x			x			x			
RL		7135														
RR		7136							x							
RSTOP		72														
SBOUND		77														
SCDR		118					x						x			
SCR		116			x		x						x			
SCRE		143			x		x						x			
SHELL		73														
SIG		7137				x										
SIGC	100	100								x						
SN		65							x							
SØLID	400	9905		x	x		x	x	x	x			x			
SUMFE		107														
SVS		103						x					x			x
SWITCH		7139														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
S1		90		x	x	x			x	x				x		
S10		99														
S2		91														
S3		92														
S4		93														
S5		94														
S6		95														
S7		96														
S8		97														
S9		98														
T		84			x	x	x						x			
TAB	15	205														
TABLM	50	7140														
TAU	52	7190		x	x		x	x	x	x			x			
TAUDTS		7242							x							
TAUDTX		7243														
TEMP	12	10305			x	x		x					x			
THETA	1200	605		x	x	x	x			x			x			
TMDZ		16														
TMXZ		17														
TMZ		9														
TØZØNE		75								x						
TRAD		63							x							
TXMAX		19														
TYMAX		20														
U	1200	7244		x	x	x			x	x			x			
UK		8444														
UL	200	205							x							

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
UR	200	205														
URR		8445							x	x						
UT		8446							x							
UTEF		8449														
UU		8447							x							
UUU		8448														
UVMAX		8450				x										
V	1200	8451		x	x	x			x	x			x			
VABOVE		9651							x	x						
VAPE		140			x			x					x			
VBLØ		9652							x							
VEL		9653							x							
VISC		83														
VK		9654														
VT		9655														
VTEF		9656														
VV		9657														
VVABOV		9658														
VVBLØ		9659														
WPS		9760														
WS		9761		x	x	x			x	x			x			
WSA		9762			x				x	x			x			
WSB		9763			x											
WSC		9764														
WSGD		86														
WSGX		87														
W2	50	9660		x	x		x	x					x			
W3	50	9710														

Table III

CROSS REFERENCE OF HECTIC VARIABLES (Continued)

	Size	Loc.	MAIN	INPUT	EDIT	CDT	SCRC	BOIL	PH1	PH2	FLAG	DJLOW	SETUP	SPRINT	ES	ESK
X	53	152		x	x		x		x	x			x			
XL		9765														
XLF		9766														
XMAX		18			x								x			
XN		9767														
XNRG		64														
XR		9768														
XX	54	151														
X1		78			x											
X2		79			x											
Y	100	1806		x	x								x			
YAMC	100	305								x						
YL		9769														
YLW		9770														
YN		9771														
YU		9772														
YY	101	1805														
Y1		80			x											
Y2		81			x											
Z	150	1		x	x	x				x			x	x		
ZMAX		9773														
IV		144			x	x										
JV		145			x	x										
IU		146			x	x										
JU		147			x	x										
DTVF		148			x	x										
DTUF		149			x	x										

2.5. APPENDIX: LISTING OF HECTIC

```
$I    FOR  MAIN, MAIN/FJ
C
C     HECTIC PROGRAM MODIFIED 7/30/66
C
C*****************************************************************************
C*****************************************************************************
C     MAIN FOR  INTER CODE
C     NOTE ---- 1 MATERIAL (X) ONLY
C
C
      CALL INPUT
C
      CALL EDIT
C
C     CALCULATES TIME STEP AND PRESSURES
   10 CALL CDT
C     SOURCE ROUTINE
      CALL SCRC
      CALL BOIL
C     VELOCITY AND ENERGY CHANGE DUE TO WORK TERMS ONLY
C
   20 CALL PH1
C
C     VELOCITY AND ENERGY  CHANGES DUE TO MASS TRANSPORT
      CALL PH2
      CALL EDIT
      GO TO 10
      END
```

```
0I    FOR  CARDS, CARDS/FJ
      SUBROUTINE CARDS                                                    CARD0010
      DIMENSION TABLE(1),CARD(7),LABLE(1),CAHD(18)
      COMMON           TABLE
      EQUIVALENCE(TABLE(1),LABLE(1))                                      CARD0030
      WRITE (6,10)                                                        CARD0050
    1 READ(5,11)IEND,LOC,NUMWPC,(CARD(I),I=1,7),CAHD(17),CAHD(18)         CARD0070
      IF(IEND.EQ.9) GO TO 15
      WRITE(6,12)CAHD(17),CAHD(18),IEND,LOC,NUMWPC,(CARD(I),I=1,NUMWPC)
      IF(IEND.EQ.1.AND.LOC.EQ.0) GO TO 3
      IF(IABS(NUMWPC-4).GT.3) GO TO 20
      DO 4 I=1,NUMWPC
      J=LOC+I-1                                                           CARD0100
      IF(IEND-2)2,5,2                                                     CARD0110
    5 LABLE(J)=IFIX(CARD(I))                                              CARD0120
      GO TO 4                                                             CARD0130
    2 TABLE(J)=CARD(I)                                                    CARD0140
    4 CONTINUE                                                            CARD0150
      IF(IEND-1)1,3,1                                                     CARD0160
    3 RETURN                                                              CARD0170
   15 READ(5,16)(CAHD(I),I=1,16)                                          CARD0180
      WRITE(6,17)(CAHD(I),I=1,16)
      GO TO 1
   20 WRITE(6,21)
      CALL EXIT
C                FORMATS
   10 FORMAT(20H1HECTIC  INPUT CARDS///)                                  CARD0190
   11 FORMAT(I1,I5,I1,0P7E9.4,2A5)
   12 FORMAT(1H 2A5,I4,I7,I3,1P7E14.6)
   16 FORMAT(16A5)
   17 FORMAT(1X,16A5)
   21 FORMAT(20X,24H THE ABOVE CARD IN ERROR)
      END
                                                                          CARD0230
```

```
W1    FOR  INPUT, INPUT/F
      SUBROUTINE  INPUT                                                    -
C                                                                          INP00020
C                D  I  M  E  N  S  I  O  N
C
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),    AIX(1200),    P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200),  CAP(1200),    KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4UX(52),    X(53),      XX(54),     DY(100),    Y(100),     YY(101),
     5TAB(15),   AMK(15),    PK(15),     GK(15),     Z(150),     ZZ(150),
     6TAU(52),   PL(200),    PR(200),    UL(200),    UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          A1D     ,AIX     ,AM      ,AMO     ,AMX     ,ARLA
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,GUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,GUOOFL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IWI     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                E  Q  U  I  V  A  L  E  N  C  E
     EQUIVALENCE      (Z,IZ,PROB),     (Z(2),CYCLE),    (Z(3),DT),
     1(Z(4),PRINTS),  (Z(5),PRINTL),   (Z(6),DUMPT7),   (Z(7),CSTOP),
     2(Z(8),PIDY),    (Z(9),TMZ),      (Z(10),SCYCLE),  (Z(11),SPROB),
     3(Z(12),GAMX),   (Z(13),ETH),     (Z(14),FFA),     (Z(15),FFB),
     4(Z(16),TMDZ),   (Z(17),TMXZ),    (Z(18),XMAX),    (Z(19),TXMAX),
     5(Z(20),TYMAX),  (Z(21),AMDM),    (Z(22),AMXM),    (Z(23),DNN),
     6(Z(24),DMIN),   (Z(25),FEF),     (Z(26),DTNA),    (Z(27),CVIS),
     7(Z(28),NPR),    (Z(29),NPRI),    (Z(30),NC),      (Z(31),NPC),
     8(Z(32),NRC),    (Z(33),IMAX),    (Z(34),IMAXA),   (Z(35),JMAX),
     9(Z(36),JMAXA),  (Z(37),KMAX),    (Z(38),KMAXA),   (Z(39),NMAX)
     0EQUIVALENCE     (Z(40),ND),      (Z(41),KDT),     (Z(42),IXMAX),
     1(Z(43),NOD),    (Z(44),NOPR),    (Z(45),NIMAX),   (Z(46),NJMAX),
     2(Z(47),I1),     (Z(48),I2),      (Z(49),I3),      (Z(50),I4),
     3(Z(51),N1),     (Z(52),N2),      (Z(53),N3),      (Z(54),N4),
     4(Z(55),N5),     (Z(56),N6),      (Z(57),N7),      (Z(58),N8),
     5(Z(59),N9),     (Z(60),N10),     (Z(61),N11),     (Z(62),NRM),
     6(Z(63),TRAD),   (Z(64),XNRG),    (Z(65),SN),      (Z(66),DXN),
     7(Z(67),RADER),  (Z(68),RADET),   (Z(69),RADER),   (Z(70),DTRAD),
     8(Z(71),REZFCT), (Z(72),RSTOP),   (Z(73),SHELL),   (Z(74),BBOUND),
     9(Z(75),TOZONE), (Z(76),ECK),     (Z(77),SBOUND),  (Z(78),X1)
     0EQUIVALENCE     (Z(79),X2),      (Z(80),Y1),      (Z(81),Y2),
     1(Z(82),CABLN),  (Z(83),VISC),    (Z(84),T),       (Z(85),GMAX),
     2(Z(86),WSGD),   (Z(87),WSGX),    (Z(88),GMADR),   (Z(89),GMAXR),
     3(Z(90),S1),     (Z(91),S2),      (Z(92),S3),      (Z(93),S4),
     4(Z(94),S5),     (Z(95),S6),      (Z(96),S7),      (Z(97),S8),
     5(Z(98),S9),     (Z(99),S10)
C
     EQUIVALENCE      (Z(100),HVB),    (Z(101),HCB),    (Z(102),CB),
```

```
     1(Z(103),SVS),     (Z(104),ATOM),     (Z(105),CV),       (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),     (Z(109),ALCO),     (Z(110),ANN),
     3(Z(111),EZERO),   (Z(112),PW),       (Z(113),CAPS),     (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),      (Z(121),IH),       (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),       (Z(125),JC),       (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),      (Z(129),HH),       (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),       (Z(133),J3),       (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                          (Z(138),SVMAX),
     8(Z(139),FRCDTC)
     1EQUIVALENCE       (Z(140),VAPE),     (Z(141),RADE),     (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),       (Z(145),JV),       (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),     (Z(149),DTUF),     (Z(150),EI1)
C
     1EQUIVALENCE       (XX(2),X(1)),      (UR,UL,FLEFT),     (UR(100),YAMC),
     1(PR(100),SIGC),   (PR,PL,GAMC),      (DKE,THETA),       (UR,TAB),
     2(UR(16),AMK),     (UR(31),PK),       (UR(46),QK),       (YY(2),Y(1))
C
C                C      O      M      M      O      N
C
C     1SEND SET EQUAL TO 1 ON THE FIRST CYCLE
C
      1SEND=1
C*********************************************************************
C     'N7' EITHER SET TO '10' (OLD DUMP TAPE) OR
C     SET TO '11' (NEW DUMP TAPE).
      N7=10
C                                                                      INPU1030
      READ(5,8004) (HEAD(I),I=1,12)
      WRITE(6,8005) (HEAD(I),I=1,12)
      CALL CARDS                                                       INPU1060
      IF(SCYCLE.GT.0.) GO TO 1000
      CALL SETUP
C                                                                      INPU1510
C                                                                      INPU1520
C**** R E A D   T A P E ***************************************************INPU1540
C                                                                      INPU1530
 1000 MZ=150
      REWIND 10
 1004 READ(10) WS,CYCLE,PROB
      IF(WS-555.)1004,1005,1004
 1005 IF(SPROB-PROB)9902,1006,9902
 1006 IF(SCYCLE-CYCLE)9903,1023,1004
 1023 READ(10)(Z(I),I=1,MZ)
      READ(10) (U(I),V(I),AMX(I),AIX(I),P(I),THETA(I),
     1 RHO(I),FIOUT(I),CAP(I),KFIT(I),I=1,KMAXA)
      READ(10) X(0),(X(I),TAU(I),I=1,IMAX)
      READ(10)(Y(I),I=0,JMAX)
 1024 IF(CYCLE)9904,1040,1025
 1025 READ(10)(W2(I),I=1,50)
      READ(10)(SOLID(I),I=1,400)
C**** END OF READ TAPE ****************************************************INPU2000
C                                                                      INPU2010
C                                                                      INPU2020
C               READ IN REMAINING INPUT CARDS                          INPU1110
 1040 CALL CARDS
C                                                                      INPU2030
C               GENERATE DX AND DY                                     INPU1330
      DO 50 I=1,IMAX
   50 DX(I)=X(I)-X(I-1)                                                INPU1350
      DO 55 J=1,JMAX                                                   INPU1360
   55 DY(J)=Y(J)-Y(J-1)                                                INPU1370
   56 IF(SCYCLE)9905,60,57
   57 WRITE(6,58) NC
   58 FORMAT(29H0  PROBLEM RESTART FROM CYCLE,I10)
```

```
   60 S1=0.0
      RETURN
C
C                    ERROR                                          INPU2200
 9902 S1=3.1005                                                     INPU2210
      GO TO 9999
 9903 S1=3.1006                                                     INPU2250
      GO TO 9999
 9904 S1=3.1024                                                     INPU2270
      GO TO 9999
 9905 S1=3.0056                                                     INPU2290
 9999 CALL EDIT
C
C                                                                   INPU2390
C                    FORMATS                                        INPU2470
 8004 FORMAT(12A6)                                                  INPU2480
 8005 FORMAT(1H1,12A6)
      END                                                           INPU2530
```

```
WI    FOR  EDIT, EDIT/FJ
      SUBROUTINE EDIT                                                    EDIT0010
C
C
C                  D  I  M  E  N  S  I  O  N
C
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),    AIX(1200),    P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200),  CAP(1200),    KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),      X(53),       XX(54),       DY(100),      Y(100),      YY(101),
     5TAB(15),     AMK(15),     PK(15),       QK(15),       Z(150),      IZ(150),
     6TAU(52),     PL(200),     PR(200),      UL(200),      UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
C
C
C                                                                        EDIT0990
C                  C     O     M     M     O     N
C
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,A
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,QOOOFL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                                                                        EDIT0920
C                  E  Q  U  I  V  A  L  E  N  C  E
C
     0EQUIVALENCE      (Z,IZ,PROB),     (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),   (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TM2),      (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),     (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),    (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),    (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),     (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),    (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),    (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),    (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),      (Z(41),KD1),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),    (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),      (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),      (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),      (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),     (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),    (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),   (Z(69),RADER),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),   (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),     (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),      (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),  SC),    (Z(84),T),        (Z(85),GMAX),
```

```
     2(Z(86),WSGD),     (Z(87),WSGA),     (Z(88),GMAOR),     (Z(89),GMAXR),
     3(Z(90),S1),       (Z(91),S2),       (Z(92),S3),        (Z(93),S4),
     4(Z(94),S5),       (Z(95),S6),       (Z(96),S7),        (Z(97),S8),
     5(Z(98),S9),       (Z(99),S10)
C
      EQUIVALENCE       (Z(100),HVB),     (Z(101),HCST),     (Z(102),CB),
     1(Z(103),SVS),     (Z(104),ATOM),    (Z(105),CV),       (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),    (Z(109),ALCO),     (Z(110),AHN),
     3(Z(111),EZERO),   (Z(112),PW),      (Z(113),CAPS),     (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCR),     (Z(117),ISR),      (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),     (Z(121),IH),       (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),      (Z(125),JC),       (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),     (Z(129),HH),       (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),       (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                         (Z(138),SYMAX),
     8(Z(139),FRCUT(,)
      EQUIVALENCE       (Z(140),VAPE),    (Z(141),RADE),     (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),      (Z(145),JV),       (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),    (Z(149),DTUF),     (Z(150),E1))
C
C
      EQUIVALENCE       (XX(2),X(1)),     (UR,UL,FLEFT),     (UR(100),YAMC),
     1(PR(100),SIGC),   (PR,PL,GAMC),     (DKE,THETA),       (UR,TAB),
     2(UR(16),AMK),     (UR(31),PK),      (UR(46),QK),       (YY(2),Y(1))
C
C
C                                                                        EDIT1000
C     ISEND = 1, FIRST CYCLE
C     ISEND = 2, INTERMEDIATE CYCLES
C     ISEND = 3, LAST CYCLE
C                                                                        EDIT1030
C                                                                        EDIT1100
C                                                                        EDIT1110
C                E D I T                                                 EDIT1120
      IGOTO=1
      GO TO(6000,101,101),ISEND
  101 IF(S1.GT.0.) GO TO 110
  108 IF(CYCLE-CSTOP)115,109,115
  109 S1=4.0108
  110 ISEND=3
C     ALL   PRINTS PLUS WRITE ON BINARY TAPE
      GO TO 6000
  115 IF(AMOD(CYCLE,PRINTS))118,117,118
C     SHORT PRINTS ONLY
  117 IGOTO=2
      GO TO 6000
  118 IF(AMOD(CYCLE,PRINTL))120,119,120
C     LONG PRINTS ONLY
  119 IGOTO=3
      GO TO 5000
  120 IF(AMOD(CYCLE,DUMPT7))126,121,126
  121 IF(IGOTO.EQ.1) GO TO 6000
      IGOTO=1
      GO TO 1
  125 IF(ISEND.EQ.3) CALL SPRINT
  126 IF(ABS(ECK).GT.DMIN) GO TO 9901
  140 RETURN
C                                                                        EDIT1500
C                                                                        EDIT1510
C**** SUBROUTINE WTAPE ***************************************************EDIT1520
C          DUMP ON TAPE N7                                               EDIT1530
C               IF DUMPT7 IS NEGATIVE  SUPPRESS ANY WRITING ON TAPE 7    EDIT1540
    1 IF(ISEND.EQ.1.AND.N7.EQ.10) GO TO 126
      IF(DUMPT7)30,3,3                                                   EDIT1550
    3 WS=555.0
```

```
      WRITE(N7) WS,CYCLE,PROB
      WRITE(N7)(Z(I),I=1,M2)
      WRITE(N7)(U(I),V(I),AMX(I),AIX(I),P(I),THETA(I),
     1 RHO(I),FIOUT(I),CAP(I),KFIT(I),I=1,KMAXA)
      WRITE(N7) X(0),(X(I),TAU(I),I=I,IMAX)
      WRITE(N7)(Y(I),I=0,JMAX)
      WRITE(N7) (W2(I),I=I,50)
      WRITE(N7)(SOLID(I),I=I,400)
      WS=666.0                                                    EDIT1730
      WRITE(N7) WS,WS,WS
      WRITE (6,8120)NC                                            EDIT1750
   30 GO TO 125
C**** END OF  WTAPE SUBROUTINE ***************************************EDIT1770
C                                                                  EDIT1780
C                                                                  EDIT1790
C**** SUBROUTINE S P *************************************************EDIT1800
 6000 NK=I2                                                        EDIT1820
 6010 DO 6012 I=1,I8                                               EDIT1950
 6012 PR(I)=0.0                                                    EDIT1960
      DO 6028 K=2,KMAX                                             EDIT2020
      WSB=(U(K)**2+V(K)**2)/2.0                                    EDIT1750
 6019 IF(AMX(K))9902,6028,6020
 6020 I=NKI                                                        EDIT2090
 6026 WS=AMX(K)                                                    EDIT2160
      PR(I)= PR(1)+AIX(K)*WS
      PR(2)= PR(2)+WSB*WS
      PR(3)= PR(2)+PR(1)
 6028 CONTINUE                                                     EDIT2230
      WSA=(ETH-PR(3))/ETH
      ECK =(WSA-DNN)/FLOAT(NPC)
      DNN=WSA                                                      EDIT2340
      NPC=0                                                        EDIT2350
      WRITE(6,8116)PROB,NC,T,DT  ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
     1IZ(144),IZ(145),IZ(146),IZ(147)
      WRITE(6,6902)  PR(1),PR(2),PR(3),VAPE,RADE,CNDE,SCRE,ETH,ECK
      PR(1)=0.
      PR(2)=0.
      PR(3)=0.
      PR(4)=0.0                                                    EDIT1780
      WRITE(6,6904)
      DO 6040  I=1,ISR
      J=(I-1)*20+1
      TEMP(1)=SOLID(J+12)/ SCR
      TEMP(2)=SOLID(J+13)/ SOLID(J+4)
      TEMP(3)=SOLID(J+6) / SCR
      TEMP(4)=SOLID(J+7) / SOLID(J+4)
      IF( SCR.NE.0.) GO TO        6030
      TEMP(1)=0.
      TEMP(3)=0.
 6030 CONTINUE
      PR(1) = PR(1) +  TAU(I)*SOLID(J+6)
      PR(2) = PR(2) +  TAU(I)*SOLID(J+7)
      PR(3) = PR(3) +  TAU(I)*SOLID(J+12)
      PR(4) = PR(4) +  TAU(I)*SOLID(J+13)
      PR(5) = PR(5) +  TAU(I)*W2(I)
      PR(6) = PR(6) +  TAU(I)*SOLID(J+8)
      PR(7) = PR(7) +  TAU(I)*SOLID(J+2)
      PR(8) = PR(8) +  TAU(I)*TEMP(1)
      PR(9) = PR(9) +  TAU(I)*TEMP(2)
      PR(10)= PR(10) + TAU(I)*TEMP(3)
      PR(11)= PR(11) + TAU(I)*TEMP(4)
      WRITE(6,6906)I,SOLID(J+6),SOLID(J+7),SOLID(J+12),SOLID(J+13),W2(I)
     1,SOLID(J+8),SOLID(J+2),TEMP(1),TEMP(2),TEMP(3),TEMP(4)
 6040 CONTINUE
      WRITE(6,6908)(PR(I),I=1,11)
```

```
C**** END OF   S P  SUBROUTINE ********************************************EDIT2920
C                                                                          EDIT2930
C                                                                          EDIT2940
C**** SUBROUTINE PLOT ******************************************************EDIT2950
 1000 CONTINUE
      WRITE(6,8116)PROB,NC,T,DT  ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
     1IZ(144),IZ(145),IZ(146),IZ(147)
      JMAX=JMAX                                                            EDIT2980
      WRITE (6,8307)X1,X2,XMAX,Y1,Y2,Y(JMAX)                               EDIT2990
      M=1                                                                  EDIT3000
      IF(JMAX-52)1034,1036,1036                                            EDIT3010
 1034 M=IABS(51-JMAX)/2                                                    EDIT3020
 1036 DO 1040 I=1,M                                                        EDIT3030
      WRITE (6,8308)                                                       EDIT3040
 1040 CONTINUE                                                             EDIT3050
 1044 J=JMAX                                                               EDIT3060
 1100 K=(J-1)*IMAX+1                                                       EDIT3070
 1105 DO 1180 I=1,IMAX                                                     EDIT3080
      K=K+1                                                                EDIT3090
 1126 PR(I)=1H
 1130 IF(J-J5-1)1136,1132,1136
 1132 IF(I-I1-1)1140,1134,1134                                             EDIT3130
 1134 IF(I-I2-1)1144,1144,1136                                             EDIT3140
 1136 IF(I-I1-1)1140,1138,1140                                             EDIT3150
 1138 IF(J-J5)1140,1140,1144
 1140 IF(I-I2-1)1150,1142,1150
 1142 IF(J-J5)1150,1150,1144
 1144 PR(I)=2H .
      GO TO 1180
C       TEST FOR X PARTICLE                                                EDIT3240
 1150 IF(AMX(K))9903,1166,1160
 1160 PR(I)=2H X
      GO TO 1180                                                           EDIT3310
 1166 PR(I)=2H
 1180 CONTINUE                                                             EDIT3420
 1200 IF(MOD(J,5))1210,1204,1210                                           EDIT3430
 1204 IF(DY(J)-DY(J-1))1206,1208,1206                                      EDIT3440
 1206 WRITE (6,8211)DY(J),J,(PR(I),I=1,IMAX)                               EDIT3450
      GO TO 1224                                                           EDIT3460
 1208 WRITE (6,8201)J,(PR(I),I=1,IMAX)                                     EDIT3470
      GO TO 1224                                                           EDIT3480
 1210 IF(DY(J)-DY(J-1))1212,1214,1212                                      EDIT3490
 1212 WRITE (6,8222)DY(J),(PR(I),I=1,IMAX)                                 EDIT3500
      GO TO 1224                                                           EDIT3510
 1214 WRITE (6,8202)(PR(I),I=1,IMAX)                                       EDIT3520
 1224 J=J-1                                                                EDIT3530
 1226 IF(J)1230,1230,1100                                                  EDIT3540
 1230 PR(I)=2H -
      WRITE (6,8201)J,(PR(1),I=1,IMAX)                                     EDIT3570
      WRITE (6,8302)(I,I=0,IMAX,5)                                         EDIT3580
 1240 GO TO(5000,118,9906),IGOTO
C**** END OF  PLOT  SUBROUTINE *********************************************EDIT3600
C                                                                          EDIT3610
C                                                                          EDIT3620
C**** SUBROUTINE L P *******************************************************EDIT3630
 5000 CONTINUE
      WRITE(6,8116)PROB,NC,T,DT  ,DTH,DTC,Z(148),Z(149),IH,JH,IC,JC,
     1IZ(144),IZ(145),IZ(146),IZ(147)
 5004 DO 5050 I=1,IMAX                                                     EDIT3700
      LPP=1
      J=JMAXA                                                              EDIT3720
      K=KMAX+I                                                             EDIT3730
      DO 5046 L=1,JMAX                                                     EDIT3740
      J=J-1                                                                EDIT3750
      K=K-IMAX                                                             EDIT3760
```

```
      YTAR=Y(J5I-Y(J)
 5012 IF(AMX(K))9904,5046,5014
 5014 GO TO(5016,5018),LPP
 5016 LPP=2
      WRITE(6,8135)I,X(I),DX(1)
 5018 WRITE(6,8108) J,U(K),V(K),P(K),THETA(K),AMX(K),
     1AIX(K),RHO(K),FIOUT(K),CAP(K),YTAR                                EDIT3830
 5046 CONTINUE                                                          EDIT3840
 5050 CONTINUE                                                          EDIT3860
 5051 GO TO(1,9905,120),IGOTO
C**** END OF   L P  SUBROUTINE ********************************************EDIT3870
C                                                                       EDIT3880
C                                                                       EDIT3890
C                ERROR
 9901 S1=4.0126
      GO TO 9999
 9902 S1=4.6019
      GO TO 9999
 9903 S1=4.1150
      GO TO 9999
 9904 S1=4.5012
      GO TO 9999
 9905 S1=4.5051
      GO TO 9999
 9906 S1=4.1240
 9999 CALL SPRINT
C                                                                       EDIT4100
C                FORMATS                                                EDIT4110
 6902 FORMAT(//6X7H1NT ENG7X,7HKIN ENG,7X,7HINT+KIN,7X,7HBVP ENG,7X,7HRA
     1D ENG,7X,7HCND ENG,7X,7HSCR ENG / 3X,1P7E14.7 //34X,7HTHE ENG,7X,
     27HREL ERR /31X1P2E14.7 //)
 6904 FORMAT(3H  I2X6HMDOT/A4X3HM/A7X6HIDOT/A4X3H1/A7X7HESDOT/A3X
     2    4HES/A6X7HEBDOT/A3X8H(I/E)DOT2X3HI/E7X7HM/E DOT3X3HM/E /)
 6906 FORMAT(13,1P11E10.3)
 6908 FORMAT(1/1X14HSUM TIMES AREA/3X1P11E10.3)
 8108 FORMAT(13,1P11E10.3)
 8116 FORMAT( 7H1  PROB5X,5HCYCLE5X,4HTIME6X,2HDT8X,3HDTH7X,
     1 3HDTC7X,4HDTVF6X,4HDTUF6X,2HIH2X,2HJH2X,2HIC2X,2HJC2X,2HIV2X,2HJV
     2 2X,2HIU2X,2HJU2X / F7.1,5X,I5,3X,1P6E10.4,814 )
 8120 FORMAT(1H0//21H TAPE 7 DUMP ON CYCLEI5////)                       EDIT4220
 8127 FORMAT(13,4(1P2E12.6,I5))                                         EDIT4300
 8128 FORMAT(3H0  2(1P2E12.6,5X))
 8135 FORMAT(1H //3H I=13,6X,6HX(1) =F12.3,6X,7HDX(1) =F12.3/ 3H  J 3X
     11HU9X,1HV9X,1HP9X,5HTHETA5X,4HMASS6X,3HA1X7X,3HRH07X,4HFLUX6X,3HCA
     2P7X,1HY /)
 8201 FORMAT(I10,2H 154A2)                                              EDIT4360
 9040 FORMAT(1H / 6I6)                                                  EDIT4370
 8202 FORMAT(10X,2H 154A2)                                              EDIT4380
 8211 FORMAT(F7.1,13,2H 154A2)                                          EDIT4390
 8222 FORMAT(F7.1,3X,2H 154A2)                                          EDIT4400
 8302 FORMAT(112,10I10)                                                 EDIT4410
 8307OFORMAT(5H X1 =1PE12.6,3X,4HX2 =E12.6,3X,6HXMAX =E12.6,6X,4HY1 =E12EDIT4420
     1.6,3X,4HY2 =E12.6,3X,6HYMAX =E12.6)                               EDIT4430
 8308 FORMAT(1H /)                                                      EDIT4440
      END                                                               EDIT4450
```

```
WT    FOR  CUT, CUT/FJ
      SUBROUTINE CUT
C
C                D  I  M  E  N  S  I  O  N
C
                        DIMENSION
     1U(1200),      V(1200),      AMX(1200),    AIX(1200),    P(1200),
     2THETA(1200), RHO(1200),    FIOUT(1200), CAP(1200),    KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),      X(53),        XX(54),       DY(100),      Y(100),      YY(101),
     5TAB(15),     AMK(5),       PK(15),       QK(15),       Z(150),      IZ(150),
     6TAU(52),     PL(200),      PR(200),      UL(200),      UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON           Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON           AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON           BIG     ,BOUNCE  ,DDXM    ,DDVK    ,DVK     ,DX
      COMMON           DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON           P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON           PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON           RR,SIG,GOODFL,SWITCH ,TABLM,TAU
      COMMON           TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON           UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON           VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON           VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON           WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON           XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON           I       ,I1      ,IN      ,IR      ,IWS     ,IWSA
      COMMON           IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON           JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON           L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON           ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON           NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON           FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                E  Q  U  I  V  A  L  E  N  C  E
C
     0EQUIVALENCE      (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),LTH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPR1),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CAULN),   (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
```

```
      EQUIVALENCE       (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
     1(Z(103),SVS),     (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANU),
     3(Z(111),EZERO),   (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
     3(Z(115),COL),     (Z(116),SCR),     (Z(117),ISR),     (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),     (Z(121),IH),      (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),     (Z(129),HN),      (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                        (Z(138),SVMAX),
     8(Z(139),FRCDTC)
      EQUIVALENCE       (Z(140),VAPL),    (Z(141),RADL),    (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),    (Z(149),DTUF),    (Z(150),E11)
C
      EQUIVALENCE       (XX(2),X(1)),     (UR,UL,FLLFT),    (UR(100),YAMC),
     1(PR(100),SIGC),   (PR,PL,GAMC),     (DKE,THETA),      (UR,TAB),
     2(UR(16),AMK),     (UR(31),PK),      (UR(46),QK),      (YY(2),Y(1))
C
C
C                 C       O       M       M       O       N
C
C
C
C     FOR 1 MATERIAL ONLY
      ISEND=2
      UVMAX=-1./DTNA**2
      TEMP(1)=-1./DTNA
      DTUF=1.E10
      DTVF=1.E10
      IF(NC.NE.0) GO TO 3005
      DTUF=DT
      DTVF=DT
 3005 DO 3280 I=1,IMAX
      DO 3280 J=1,JMAX
      K=(J-1)*IMAX+I+1
 3004 IF(AMX(K))9901,3260,3025
 3025 SV=1./RHO(K)
      IF(JMR(KF1T(K),2).EQ.0) GO TO 3260
      IF(P(K).LE.1.E-20) P(K)=0.
      IF(SV.GT.Z(138)) GO TO 3280
      SIG=DX(1)
      IF(DY(J).GT.SIG) GO TO 3140
      SIG=DY(J)
 3140 WS=(P(K)+SV)*(1.0+(P(K)*SV)/A1X(K))
 3205 DTC=WS/SIG**2
      IF(UVMAX.GT.DTC)GO TO 3220
      IC=I
      JC=J
      UVMAX=DTC
 3220 DTH=ABS(U(K))/DX(1)
 3225 IF(TEMP(1).GT.DTH)GO TO 3235
      IH=I
      JH=J
      TEMP(1)=DTH
 3235 DTH=ABS(V(K))/DY(J)
 3240 IF(TEMP(1).GT.DTH)GO TO 3280
      IH=I
      JH=J
      TEMP(1)=DTH
      GO TO 3280
 3260 IF(P(K).EQ.0.) GO TO 3270
      TEMP(2)= DY(J)/ABS(P(K))*.25
      IF(TEMP(2).GT.DTVF) GO TO 3270
      DTVF=TEMP(2)
```

```
      IV=I
      JV=J
 3270 IF(THETA(K).EQ.0.) GO TO 3280
      TEMP(3)=DX(I)/ABS(THETA(K))*.25
      IF(TEMP(3).GT.DTUF) GO TO 3280
      DTUF=TEMP(3)
      IU=I
      JU=J
 3280 CONTINUE
      DTNA=DT
      DTH=Z(139)/ABS(TEMP(1))
      DTC=1./SQRT(ABS(UVMAX))
      DT=AMIN1(AMIN1(AMIN1(AMIN1(DTNA*FFA,DTC),DTH),DTVF),DTUF)
 3029 IF(DT.LT.FFB) GO TO 9902
 3290 IF(T.LT.0.) GO TO 9903
 3300 T=T+DT
      NC=NC+1
      CYCLE=NC
      NPC=NPC+1
       RETURN
C                NEGATIVE MASS
 9901 S1=5.3004
      GO TO 9999
 9902 S1=5.3029
      GO TO 9999
 9903 S1=5.3290
 9999 CALL EDIT
      END
```

```
WI    FOR  SCRC, SCRC/FU                                                    -
      SUBROUTINE SCRC
C                 D   I   M   E   N   S   I   O   N                        0 D0050
C                                                                          0 D0060
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),     X(53),     XX(54),     DY(100),    Y(100),     YY(101),     0 D0110
     5TAB(15),    AMK(15),   PK(15),     QK(15),     Z(150),     IZ(150),     0 D0120
     6TAU(52),    PL(200),   PR(200),    UL(200),    UR(200),                 0 D0130
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),                              0 D0140
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON           Z      ,XX     ,UR     ,PR     ,THETA  ,YY           0 D0160
      COMMON           AID    ,AIX    ,AM     ,AMD    ,AMX    ,AREA         0 D0170
      COMMON           BIG    ,BOUNCE ,DDXN   ,DDVK   ,DVK    ,DX           0 D0180
      COMMON           DY     ,E      ,FD     ,FS     ,FX     ,OUT          0 D0190
      COMMON           P      ,PABOVE ,PBLO   ,PIDTS  ,PPABOV ,PRR          0 D0200
      COMMON           PUL    ,QDT    ,RC     ,REZ    ,RHO    ,RL           0 D0210
      COMMON           RR,SIG,GOODFL,SWITCH ,TABLM,TAU                       0 D0220
      COMMON           TAUDTS ,TAUDTX ,U      ,UK     ,URR    ,UT           0 D0230
      COMMON           UU     ,UUU    ,UTEF   ,UVMAX  ,V      ,VABOVE       0 D0240
      COMMON           VBLO   ,VEL    ,VK     ,VT     ,VTEF   ,VV           0 D0250
      COMMON           VVABOV ,VVBLO  ,W2     ,W3     ,WPS    ,WS           0 D0260
      COMMON           WSA    ,WSB    ,WSC    ,XL     ,XLF    ,XN           0 D0270
      COMMON           XR     ,YL     ,YLW    ,YN     ,YU     ,ZMAX         0 D0280
      COMMON           I      ,II     ,IN     ,IR     ,IWS    ,IWSA         0 D0290
      COMMON           IWSB   ,IWSC   ,IW1    ,J      ,JN     ,JP           0 D0300
      COMMON           JR     ,K      ,KN     ,KP     ,KR     ,KRM          0 D0310
      COMMON           L      ,M      ,MA     ,MB     ,MC     ,MD           0 D0320
      COMMON           ME     ,MZ     ,N      ,NK     ,NKMAX  ,NK1          0 D0330
      COMMON           NO     ,NR     ,G      ,SOLID  ,TEMP                 0 D0340
      COMMON           FIOUT  ,CAP    ,KFIT   ,ISEND  ,IGOTO  ,HEAD
C                                                                          0 D0440
C                                                                          0 D0450
C                 E   Q   U   I   V   A   L   E   N   C   E
C
     UEQUIVALENCE      (Z,IZ,PROB),     (Z(2),CYCLE),    (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),   (Z(6),DUMPT7),   (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),      (Z(10),SCYCLE),  (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),     (Z(14),FFA),     (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),    (Z(18),XMAX),    (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),    (Z(22),AMXM),    (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),     (Z(26),DTNA),    (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),    (Z(30),NC),      (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),    (Z(34),IMAXA),   (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),    (Z(38),KMAXA),   (Z(39),NMAX)
     UEQUIVALENCE      (Z(40),ND),      (Z(41),KDT),     (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),    (Z(45),NIMAX),   (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),      (Z(49),I3),      (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),      (Z(53),N3),      (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),      (Z(57),N7),      (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),     (Z(61),N11),     (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),    (Z(65),SN),      (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),   (Z(69),RADEB),   (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),   (Z(73),SHELL),   (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),     (Z(77),SBOUND),  (Z(78),X1)
     UEQUIVALENCE      (Z(79),X2),      (Z(80),Y1),      (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),    (Z(84),T),       (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),    (Z(88),GMADR),   (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),      (Z(92),S3),      (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),      (Z(96),S7),      (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
     UEQUIVALENCE      (Z(100),HVB),    (Z(101),HCB),    (Z(102),CB),
```

```
      1(Z(103),SVS),     (Z(104),ATOM),     (Z(105),CV),       (Z(106),GV),
      2(Z(107),SUMFL),   (Z(108),BETA),     (Z(109),ALCO),     (Z(110),ANN),
      3(Z(111),LZERO),   (Z(112),PW),       (Z(113),CAPS),     (Z(114),HNU),
      4(Z(115),COE),     (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCDR),
      5(Z(119),AHN),     (Z(120),DTH),      (Z(121),IH),       (Z(122),JH),
      6(Z(123),DTC),     (Z(124),IC),       (Z(125),JC),       (Z(126),RFT),
      X(Z(127),CDUT),    (Z(128),HCP),      (Z(129),HH),       (Z(130),CO),
      6(Z(131),J1),      (Z(132),J2),       (Z(133),J3),       (Z(134),J4),
      7(Z(135),J5),      (Z(136),J6),                          (Z(138),SVMAX),
      8(Z(139),FRCDTC)
      DEQUIVALENCE       (Z(140),VAPE),     (Z(141),RADE),     (Z(142),CNDE),
      1(Z(143),SCRE),    (Z(144),IV),       (Z(145),JV),       (Z(146),IO),
      2(Z(147),JO),      (Z(148),DTVF),     (Z(149),DTUF),     (Z(150),EI14
C
      DEQUIVALENCE       (XX(2),X(1)),      (UR,UL,FLEFT),     (UP(100),YAMC),  0 D0750
      1(PR(100),SIGC),   (PR,PL,GAMC),      (DKE,THETA),       (UR,TAB),        0 D0760
      2(UR(16),AMK),     (UR(31),PK),       (UR(46),QK),       (YY(2),Y(1))     0 D0770
C                                                                               0 D0740
C                                                                               0 D0780
C                                                                               0 D0790
C                C       O       M       M       O       N                    0 D0800
C                                                                               0 D0810
C                                                                               0 D0950
C                                                                               0 D1020
C     W2(I)      W2(I)      FLUX INTO SOLID
C     Z(115)     COE        ABSORPTION COEF.     (CM**2/GM)
C     Z(116)     SCR        INITIAL SOURCE       (JERK/CM**2-SH)
C     Z(117)     ISR        NO. OF ZONES WITH SOURCE IN I DIRECTION
C     Z(118)     SOURCE DURATION
      F1FT1=EZERO
      IF( NC.EQ.1)
     1F1FT=0.5*EZERO*(2.*(T-DT)/SCDR)**(ANN+1.)
      IF(T.LT.0.5*SCDR) GO TO 1
      IF(T.GT.SCDR) GO TO 2
      FIFT1=EZERO*(1.-.5*(2.*(1.-T/SCDR))**(ANN+1.))
      GO TO 2
    1 F1FT1=0.5*EZERO*(2.*T/SCDR)**(ANN+1.)
    2 SCR=ABS(FIFT1-FIFT)/DT
      FIFT=FIFT1
      SCRE = FIFT* PIDY*X(ISR)**2
      IF((T.GE.SCDR).AND.((T-DT).LE.SCDR)) SCR =0.
      I4P=J5+1
      DO 200  I=1,ISR
      IS=(I-1)*20+1
      SOLID(IS+4)=FIFT
      DF1S=0.
      FIIN = SCR
      W2(I)=0.
      DO 100 J=2,I4P
      K=(J-1)*IMAX+I+1
      N=K-1MAX
      IF(J.EQ.I4P) GO TO 20
      IF(JMR(KF1T(K),2).NE.1) GO TO 100
      IF(JMR(KFIT(N),2).NE.1) GO TO 50
      IF( J.EQ.2) F1OUT(N)=F11N
      IF(SCDR.EQ.0.) FIOUT(K)=0.
   20 FIIN=FIOUT(N)
      IF(J.EQ.I4P) GO TO 50
   50 SV=1./RHO(K)
      CALL ESK(THETA(K),SV,N,CAP(K))
      ROSC=-RHO(K)*DY(J)*CAP(K)
      IF(ROSC.NE.0.) GO TO 65
      FIOUT(K)=FI1N
      DFI=0.
      GOTO 70
```

```
   65 CONTINUE
      FIOUT(K)=FIIN*EXP(ROSC)
      DFI=FIIN-FIOUT(K)
      GO TO 70
   60 W2(I)=FIIN
      DFI=0.
   70 DFIS=DFIS+DFI *DT*TAU(I)
      AIX(K) =AIX(K) +DFI*TAU(I)/AMX(K)*DT
  100 CONTINUE
      ETH=ETH +DFIS
  200 CONTINUE
      RETURN
      END
```

```
01    FOR  BOIL, BOIL/PJ
      SUBROUTINE BOIL
C                 D   I   M   E   N   S   I   O   N
C
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),    X(53),     XX(54),    DY(100),   Y(100),    YY(101),
     5TAU(15),   AMK(15),   PK(15),    QK(15),    Z(150),    IZ(150),
     6TAU(52),   PL(200),   PR(200),   UL(200),   UR(200),
     7FLLFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON          BIG     ,BOUNCE  ,DELTN   ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,QUODEL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,WS      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                 E   Q   U   I   V   A   L   E   N   C   E
C
     0EQUIVALENCE      (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
     0EQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
```

```
     1(Z(103),SVS),     (Z(104),ATOM),     (Z(105),CV),       (Z(106),GV),
     2(Z(107),SUMFL),   (Z(108),BETA),     (Z(109),ALCO),     (Z(110),ANN),
     3(Z(111),EZERO),   (Z(112),PW),       (Z(113),CAPS),     (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),      (Z(121),HH),       (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),       (Z(125),JC),       (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),      (Z(129),HH),       (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),       (Z(133),J3),       (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                          (Z(138),SVMAX),
     8(Z(139),FRCDTC)
     0EQUIVALENCE       (Z(140),VAPE),     (Z(141),RADE),     (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),       (Z(145),JV),       (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),     (Z(149),DTUF),     (Z(150),EII)
     0EQUIVALENCE       (XX(2),X(1)),      (UR,UL,FLEFT),     (UR(100),YAMC),
     1(PR(100),SIGC),   (PR,PL,GAMC),      (DKE,THETA),       (UR,TAB),
     2(UR(16),AMK),     (UR(31),PK),       (UR(46),QK),       (YY(2),Y(1))
C
C
C
C
C
C    CONTINUOUS BOILING VERSION
     CNDE=0.
     DO 1000 I=1,ISR
     J=J5
  10 K=(J5-1)*IMAX+I+1
     J=(I-1)*20+1
C    SOLID(J+2)=PHI SUB(SV) SUP(N+1/2)
     TEMP(1)=CDUT*HCB/(SOLID( J+1)*CV)
     IF(CDUT.EQ.0.) TEMP(1)=HCB*W2(I)/HH
     SOLID(J+2)=W2(I)-TEMP(1)
     IF(SOLID(J+2).GT.0.) GO TO 20
     SOLID(J+2) =0.
     SOLID(J+6) =0.
     SOLID(J+12)=P(K)
     SOLID(J+11)=0.
     SOLID(J+14)=0.
     SOLID(J+15)=0.
     GO TO 450
  20 CONTINUE
C    P TEST
     SOLID(J+11)=SOLID(J+2)*CO/(GV*(HH-HCB))
 200 L=K-IMAX
     SOLID(J+10)=P(K)
     IF(JMR(KFIT(L),2).NE.1) GO TO 210
     IF(P(L).GE.P(K))GO TO 210
     SOLID(J+10)=(3.*P(K)-P(L))/2.
 210 IF(SOLID(J+11).LT.SOLID(J+10)) GO TO 300
C    M DOT
     SOLID(J+6)=SOLID(J+11)*GV/CO
C    VELOCITY V1
     SOLID(J+15)=-CO
     SOLID(J+12)=SOLID(J+11)+SOLID(J+6)*ABS(SOLID(J+15) )
     GO TO 450
 300 IF(SOLID(J+10).GE.(GV-1.)*HCP/SVS)GO TO 400
     AA=HVB+(GV-1.)*HCP-SOLID(J+10)*SVS
     BB=.5*((GV-1.)*HCP/SOLID(J+10)-SVS)**2
     TBB=2.*BB
     AAP=(AA/SOLID(J+2))**2
     IF(BB.GT.1.E-2*AA*AAP)GO TO 340
     SOLID(J+6)=SOLID(J+2)/AA*(1.-BB/(AA*AAP))
     GO TO 360
 340 BBP=.5*SOLID(J+2)/BB
     SBA=SQRT(1.+AA*AAP/(6.75*BB))
     SAA=(SBA+1.)*BBP
```

```
      SAA=(SBA+1.)*BBP
      SBB=(SBA-1.)*BBP
      IF(SBB.LT.0.) GO TO 350
      SOLID(J+6)=SAA**.33333-SBB**.33333
      GO TO 360
  350 SBB=-SBB
      SOLID(J+6)=SAA**.33333+SBB**.33333
  360 CONTINUE
      SOLID(J+15)=-SQRT(TBB)* SOLID(J+6)
      SOLID(J+12)=SOLID(J+10)+SOLID(J+6)*ABS(SOLID(J+15) )
      GO TO 450
  400 SOLID(J+10)=0.
      SOLID(J+6)= W2(I)/(HVB+HCB)
      SOLID(J+12)=SOLID(J+10)
  450 SOLID(J+14)=SOLID(J+6)*TAU(I)*DT
      IF(SOLID(J+2).LE.0.) GO TO 460
      SOLID(J+3)=SOLID(J+3)-HCB*SOLID(J+1)/SVS
      GO TO 465
  460 SOLID(J+3) =SOLID(J+3) +W2(I)*DT
      SOLID(J+1)=SOLID(J+1) +W2(I)*DT*SVS/HCB
      GO TO 470
  465 CONTINUE
C     SOLID(J+1)=Z(N+1)
      WMDOT=(W2(I)-SOLID(J+6)*HH)*SVS*DT/HCB
      IF(WMDOT.LT.0.) WMDOT=0.
      SOLID(J+1)=SOLID(J+1)+WMDOT
      TEMP(1)=CDUT/(CV*SOLID(J+6))
      IF(SOLID(J+1).GE.TEMP(1)) SOLID(J+1)=TEMP(1)
      SOLID(J+3) =SOLID(J+3) +HCB*SOLID(J+1)/SVS
  470 CONTINUE
      SOLID(J+7) =SOLID(J+7) +SOLID(J+6)*DT
      SOLID(J+8) =SOLID(J+8) +W2(I)*DT
      SOLID(J+13)=SOLID(J+13)+SOLID(J+12)*DT
      VAPE = SOLID(J+2)*TAU(I)*DT +VAPE +HCB*SOLID(J+14)
      CNDE=SOLID(J+3)*TAU(I)+CNDE
  500 CONTINUE
 1000 CONTINUE
 8001 RETURN
      END
```

```
WI    FOR  PH1, PH1/FJ                                                    -
      SUBROUTINE PH1                                                      PH1 0010
C                 D   I   M   E   N   S   I   O   N                     PH1 0020
C                                                                         PH1 0030
                        DIMENSION
     1U(1200),      V(1200),      AMX(1200),   AIX(1200),    P(1200),
     2THETA(1200), RHO(1200),    FIOUT(1200), CAP(1200),    KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),     X(53),      XX(54),     DY(100),     Y(100),     YY(101),   PH1 0080
     5TAB(15),    AMK(15),    PK(15),     QK(15),      Z(150),     IZ(150),   PH1 0090
     6TAU(52),    PL(200),    PR(200),    UL(200),     UR(200),               PH1 0100
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),                              PH1 0110
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON           Z       ,XX      ,UR      ,PR      ,THETA   ,YY       PH1 0130
      COMMON           AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA     PH1 0140
      COMMON           BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX       PH1 0150
      COMMON           DY      ,E       ,FD      ,FS      ,FX      ,OUT      PH1 0160
      COMMON           P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR      PH1 0170
      COMMON           PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL       PH1 0180
      COMMON           RR,SIG,QUOOFL,SWITCH ,TABLM,TAU                       PH1 0190
      COMMON           TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT       PH1 0200
      COMMON           UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE   PH1 0210
      COMMON           VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV       PH1 0220
      COMMON           VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS       PH1 0230
      COMMON           WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN       PH1 0240
      COMMON           XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX     PH1 0250
      COMMON           1       ,II      ,IN      ,IR      ,IWS     ,IWSA     PH1 0260
      COMMON           IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP       PH1 0270
      COMMON           JR      ,K       ,KN      ,KP      ,KR      ,KRM      PH1 0280
      COMMON           L       ,M       ,MA      ,MB      ,MC      ,MD       PH1 0290
      COMMON           ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1      PH1 0300
      COMMON           NO      ,NR      ,G       ,SOLID   ,TEMP             PH1 0310
      COMMON           FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C                                                                         PH1 0410
C                                                                         PH1 0420
C                 E   Q   U   I   V   A   L   E   N   C   E
C
     0EQUIVALENCE      (Z,12,PROB),     (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),   (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),      (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),     (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),    (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),    (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),     (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPR1),    (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),    (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),    (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),      (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),    (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),      (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),      (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),      (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),     (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),    (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADLT),   (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),   (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),     (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),      (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),    (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGO),    (Z(87),WSGX),    (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),      (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),      (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
     0EQUIVALENCE      (Z(100),HVB),    (Z(101),HCB),     (Z(102),CB),
```

```
     1(Z(103),SVS),     (Z(104),ATOM),     (Z(105),CV),       (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),HETA),     (Z(109),ALCO),     (Z(110),ANU),
     3(Z(111),EZERO),   (Z(112),PW),       (Z(113),CAPS),     (Z(114),HNU),
     5(Z(115),COE),     (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCUR),
     4(Z(119),AHN),     (Z(120),DTH),      (Z(121),IH),       (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),       (Z(125),JC),       (Z(126),RFT),
     X(Z(127),CUUT),    (Z(128),HCP),      (Z(129),HH),       (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),       (Z(133),J3),       (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                          (Z(138),SVMAX),
     8(Z(139),FRCDTC)
     DEQUIVALLENCE      (Z(140),VAPE),     (Z(141),RADE),     (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),       (Z(145),JV),       (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),     (Z(149),DTUF),     (Z(150),EI1)
C                                                                          PH1 0710
     DEQUIVALENCE       (XX(2),X(1)),      (UR,UL,FLEFT),     (UR(100),YAMC),PH1 0720
     1(PR(100),SIGC),   (PK,PL,GAMC),      (DKE,THETA),       (UR,TAB),      PH1 0730
     2(UR(16),AMK),     (UR(51),PK),       (UR(46),GK),       (YY(2),Y(1))   PH1 0740
C                                                                          PH1 0750
C                                                                          PH1 0760
C              C     O     M     M     O     N                             PH1 0770
C                                                                          PH1 0780
C                                                                          PH1 0920
C                                                                          PH1 1060
C                                                                          PH1 1070
C            VELOCITIES  AND  INTERNAL ENERGY FOR PHASE ONE                PH1 1080
      UU=1.0E+15
      UT=0.0
 8000 TEL=1.0
 3301 RC=DX(I)/2.0
      RR=(X(I)+X(2))/2.0
 3304 DO 3360 I=1,IMAX
      TAUDTS=TAU(I)*DT
C
C     DETERMINE LIMITS ON J LOOP
      CALL DJLOW(JLOW,JHIGH)
C
      K=I+1+(JLOW-1)*IMAX
      DO 3348 J=JLOW,JHIGH
      FI=0.
      KB=K-IMAX
      N=K+IMAX
      PIDTS=1.0/(PIDY*DT*DY(J))
C     DOES CELL CONTAIN ACTIVE MASS
   10 IF(JMR(KFIT(K),2))9901,3340,20
C     DETERMINE LOCATION IN GRID FORM I,J(I.E.KFLAG)
   20 KFLAG=JMR(KFIT(K),1)
C     COMPUTATION OF PRESSURE AND VELOCITY AT RIGHT INTERFACE
C     AND ASSOCIATED ENERGY CHANGES.
C
      GO TO(80,80,80,60,80,80,80,80,60,60,80,40,80,40,40,80),KFLAG
C     RIGHT TRANSMITTING INTERFACE AND ASSOCIATED TOTAL ENERGY CHANGE
   40 PRR=PL(J)
      URR=U(K)*RC
      ETH=ETH-(PRR*U(K)*RC)/PIDTS
      GO TO 110
C     REFLECTION AT RIGHT BOUNDARY.
   60 PRR=P(K)
      URR=0.0
      GO TO 110
C     NORMAL RIGHT INTERFACE COMPUTATION
   80 IF(JMR(KFIT(K+1),2))9902,107,106
  106 PRR=(P(K)+P(K+1))/2.0
      URR=(U(K)*RC+U(K+1)*RR)/2.0
      GO TO 110
  107 URR=U(K)*RC
```

```
      PRR=0.0
C     COMPUTATION OF PRESSURE AND VELOCITY AT TOP INTERFACE
C     OF CELL AND ASSOCIATED ENERGY CHANGE.
  110 GO TO(160,160,140,160,160,160,120,140,140,160,160,160,120,120,160,
     1160),KFLAG
C     TRANSMITTING CONDITION AT TOP CELL INTERFACE AND ASSOCIATED
C     ENERGY LOSS
  120 PABOVE=PBLO
      VABOVE=V(K)
      ETH=ETH-(PABOVE*V(K)*TAUDTS)/2.0
      GO TO 200
C     REFLECTION AT TOP INTERFACE OF CELL
  140 JB=(I-1)*20+1
      IF(I.GT.ISR) GO TO 150
      IF(SOLID(JB+2).EQ.0.) GO TO 150
      PT=AMAX1(SOLID(JB+11),AMAX1((3.*P(K)-P(KH))/2.0,P(K))    )
      IF(JMR(KFIT(KH),2).EQ.0) PT=SOLID(JB+11)
  145 PABOVE=PT
      T1=   PT         *(V(K)- SOLID(JB+15))/2.0
      VABOVE= V(K)
      ETH=ETH-     PT       *SOLID(JB+15)*TAUDTS/ 2.0
      GO TO 200
  150 PABOVE=P(K)
      VABOVE=0.0
      GO TO 200
C     NORMAL CALCULATION AT TOP INTERFACE
  160 IF(JMR(KFIT(N),2))9903,186,185
  185 PABOVE=(P(K)+P(N))/2.0
      VABOVE=(V(K)+V(N))/2.0
      GO TO 200
  186 PABOVE=0.0
      VABOVE=V(K)
C     DETERMINE IF THERE ARE BOUNDARY CONDITIONS
C     AT THE LEFT AND BOTTOM INTERFACES.
  200 GO TO(3328,220,3328,3328,320,340,3328,220,3328,320,220,3328,220,
     13328,340,220),KFLAG
C     REFLECTION AT LEFT INTERFACE OF CELL
  220 PL(J)=P(K)
      UL(J)=0.0
C     DETERMINE BOUNDARY CONDITIONS AT BOTTOM INTERFACE
      GO TO(3328,3328,3328,3328,320,340,3328,3328,3328,320,320,
     13328,3328,3328,340,340),KFLAG
C     REFLECTION AT BOTTOM INTERFACE
  320 PBLO=P(K)
      VBLO=0.0
      GO TO 3328
C     TRANSMITTIVE AT BOTTOM INTERFACE
  340 PBLO=PABOVE
      VBLO=V(K)
      ETH=ETH+(PABOVE*V(K)*TAUDTS)/2.0
C     VEL=1, FIRST PASS
 3328 IF(VEL)9904,3327,3326
 3326 CONTINUE
      V(K)=V(K)+(PBLO-PABOVE)/AMX(K)*TAUDTS                          PH1 1800
      IF(ABS(V(K)).LT.1.E1) V(K)=0.
 3329 U(K)=U(K)+(PL(J)-PRR)/AMX(K)*RC/PIDTS*2.0                      PH1 1830
      IF(ABS(U(K)).LT.1.E1) U(K)=0.
 3327 AIP=P(K)*((TAUDTS/2.0)*(VBLO-VABOVE)                          PH1 1860
     1 +(1.0/PIDTS)*(UL(J)-URR))                                    PH1 1870
C     T1 IS ZERO EXCEPT AT J=JS
      AIP=AIP+TAUDTS *T1
      WSX =AIX(K)+AIP/AMX(K)
 1000 IF(WSX)1011,1001,1001                                         PH1 1900
 1001 AIX(K)=WSX
      GO TO 3342
```

```
 1011 UT=1.0                                                          PH1 1930
      WSA=2.0*AIX(K)/3.0*UT/(AIX(K)-WSX)                              PH1 1940
 1013 IF(WSA-UU)1014,1001,1001                                        PH1 1950
 1014 UU=WSA                                                          PH1 1960
      GO TO 1001                                                      PH1 1970
 3340 PRR=0.0                                                         PH1 1980
      PABOVE=0.0                                                      PH1 1990
      URR=U(K+1)*RR                                                   PH1 2000
      VABOVE=V(N)                                                     PH1 2010
 3342 VBLO=VABOVE                                                     PH1 2020
      PL(J)=PRR                                                       PH1 2030
      UL(J)=URR                                                       PH1 2040
      K=N                                                             PH1 2050
 3348 PBLO=PABOVE                                                     PH1 2060
 3355 RC=RR                                                           PH1 2070
      RR=(X(I+1)+X(I+2))/2.0                                          PH1 2080
 3360 CONTINUE                                                        PH1 2090
 3361 IF(VEL)9905,7040,3363
 3363 VEL=0.0                                                         PH1 2110
      GO TO 3301                                                      PH1 2120
C                 ERROR                                              PH1 2130
 9901 S1=8.0010
      GO TO 9999
 9902 S1=8.0080
      GO TO 9999
 9903 S1=8.0160
      GO TO 9999
 9904 S1=8.3328
      GO TO 9999
 9905 S1=8.3361
 9999 CALL EDIT
C      NOTE, IF SN=0. CODE WILL INTEGRATE
C      BACKWARDS TO CORRECT THE INTEGRATION OF
C      INTERNAL ENERG, IF SN NOT 0. NEGATIVE
C      ENERGIES ARE LEFT ALONE.
 7040 IF(SN)7030,7031,7030
 7031 IF(UT)7020,7030,7010
 7010 UT=-1.
      UT=-UT                                                          PH1 2270
      GO TO 8000                                                      PH1 2280
 7020 UT=0.
      UT=UU                                                           PH1 2300
      NRI=UT/TRAD+1.
      NR=MIN0(NRM,NRI)
      WS=NR
      TRAD=UT/WS                                                      PH1 2330
      UTNA=UT                                                         PH1 2340
      GO TO 8000                                                      PH1 2350
 7030 RETURN
      END
```

```
UI    FOR  PH2, PH2/FJ                                                    -
      SUBROUTINE PH2                                                      PH2 0010
C
C                 D  I  M  E  N  S  I  O  N
C
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4UX(52),    X(53),      XX(54),    DY(100),    Y(100),    YY(101),
     5TAB(15),   AMK(15),    PK(15),    QK(15),     Z(150),    IZ(150),
     6TAU(52),   PL(200),    PR(200),   UL(200),    UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8B(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,QUOOFL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                 E  Q  U  I  V  A  L  E  N  C  E
C
     0EQUIVALENCE       (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),    (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),      (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),     (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),     (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),    (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),     (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),      (Z(29),NPRI),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),      (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),    (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE       (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),      (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),       (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),       (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),       (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),       (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),     (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),    (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),   (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),DBOUND),
     9(Z(75),TOZONE),   (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE       (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),    (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),     (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),       (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),       (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),       (Z(99),S10)
C
```

```
      EQUIVALENCE      (Z(100),HVB),    (Z(101),HCB),    (Z(102),CH),
     1(Z(103),SVS),    (Z(104),ATOM),   (Z(105),CV),     (Z(106),GV),
     2(Z(107),SUMFE),  (Z(108),BETA),   (Z(109),ALCO),   (Z(110),ANN),
     3(Z(111),EZERO),  (Z(112),PW),     (Z(113),CAPS),   (Z(114),HNU),
     3(Z(115),COE),    (Z(116),SCR),    (Z(117),1SR),    (Z(118),SCDR),
     4(Z(119),AHN),    (Z(120),DTH),    (Z(121),1H),     (Z(122),JH),
     5(Z(123),DTC),    (Z(124),IC),     (Z(125),JC),     (Z(126),RFT),
     X(Z(127),CDUT),   (Z(128),HCP),    (Z(129),HH),     (Z(130),CO),
     6(Z(131),J1),     (Z(132),J2),     (Z(133),J3),     (Z(134),J4),
     7(Z(135),J5),     (Z(136),J6),                      (Z(138),SVMAX),
     8(Z(139),FRCDTC)
      EQUIVALENCE      (Z(140),VAPE),   (Z(141),RADE),   (Z(142),CNDE),
     1(Z(143),SCRE),   (Z(144),IV),     (Z(145),JV),     (Z(146),IU),
     2(Z(147),JU),     (Z(148),DTVF),   (Z(149),DTUF),   (Z(150),EII)
C
      EQUIVALENCE      (XX(2),X(1)),    (UR,UL,FLEFT),   (UR(100),YAMC),
     1(PR(100),SIGC),  (PR,PL,GAMC),    (DKE,THETA),     (UR,TAB),
     2(UR(16),AMX),    (UR(31),PK),     (UR(46),QK),     (YY(2),Y(1))
C
C
C                C     O     M     M     O     N
C
C
C     ************************
C     CONTINUOUS EULERIAN TRANSPORT FOR INTER CODE
C     ************************
C     ************************
C                                                                    PH2 0740
C                                                                    PH2 0760
C                                                                    PH2 0900
C                                                                    PH2 0980
C     ==============================================                 PH2 0990
C                                                                    PH2 1010
C     FOR TEST OF MASS TRANSPORT ONLY
C
      DONNER=0.0
      DONER=0.0
C
      NRT=0
      PIDTS=1.0/(PIDY*DT)                                          PH2 1060
  101 DO 103 J=1,JMAX                                              PH2 1070
  102 GAMC(J)=0.0                                                  PH2 1080
      FLEFT(J)=0.0                                                 PH2 1090
      YAMC(J)=0.0                                                  PH2 1100
      SIGC(J)=0.0                                                  PH2 1110
  103 CONTINUE                                                     PH2 1120
      DO 547 I=1,IMAX
      CALL DJLOW(JLOW,JHIGH)
      K=1+I+(JLOW-1)*IMAX
      DO 546 J=JLOW,JHIGH
      FSR=0.
      FSB=0.
      L=K+IMAX
      LP=L+IMAX
      KB=K-IMAX
      IS=(I-1)*20+1
C     DETERMINE BOUNDARY CONDITION ON CELL I,J
      KFLAG=JMN(KFIT(K),1)
C     TEST BOUNDARY CONDITION AT BOTTOM CELL INTERFACE
      GO TO(301,99,301,301,81,82,301,99,301,81,81,301,99,301,82,
     182),KFLAG
C     REFLECTION AT BOTTOM INTERFACE
   81 IF(V(K))85,84,84
   84 AMMY=0.0
      AMMU=0.0
```

```
      AMMV=0.0
      DELEB=0.0
      GO TO 99
   85 AMMY=(AMX(K)*V(K)*DT)/DY(J)
      IF(AMMY+AMX(K))97,106,106
   97 AMMY=-AMX(K)
  106 AMMV=2.0*AMMY*V(K)
      AMMY=0.0
      AMMU=0.0
      DELEB=0.0
      GO TO 99
C     TRANSMITTIVE AT BOTTOM INTERFACE
   82 IF(V(K).EQ.0.) GO TO 84
      AMMU=AMMY*U(K)
      AMMV =AMMY*V(K)
      DELEB =AIX(K)+ (U(K)**2 +V(K)**2)/2.
      ETH =ETH + AMMY*DELEB
C     TEST BOUNDARY CONDITION AT LEFT CELL INTERFACE
   99 GO TO(301,105,301,301,301,301,301,105,301,301,105,
     )301,105,301,301,105),KFLAG
C     REFLECT AT LEFT INTERFACE OF CELL
  105 IF(U(K))108,107,107
  107 FLEFT(J)=0
      GO TO 767
  108 GAMC(J)=(AMX(K)*X(I)*2.0*U(K))/(TAU(I)*PIDTS)
      IF(GAMC(J)+AMX(K))765,766,766
  765 GAMC(J)=-AMX(K)
  766 FLEFT(J)=2.0*GAMC(J)*U(K)
  767 GAMC(J)=0.0
      YAMC(J)=0.0
      SIGC(J)=0.0
C     TOP INTERFACE OF CELL COMPUTATION
  501 GO TO(304,304,302,304,304,304,303,302,302,304,
     1304,304,303,303,304,304),KFLAG
C     REFLECT AT TOP CELL INTERFACE
  302 IF((I.GT.ISR) .OR. (SOLID(IS+2).EQ.0.)) GO TO 3302
      AMPY=-SOLID(IS+14)
      IF(AMPY.EQ.0.) GO TO 501
      GO TO 503
 3302 IF(V(K)) 305,305,306
  305 AMVT=0.0
      GO TO 501
  306 AMPY=(AMX(K)*V(K)*DT)/DY(J)
      IF(AMPY+AMX(K))307,308,308
  307 AMPY=-AMX(K)
  308 AMVT=2.0*AMPY*V(K)
  501 AMPY=0.0
      AMUT=0.0
      DELET=0.0
      GO TO 503
C     TRANSMIT AT TOP CELL INTERFACE
  303 IF(V(K))504,504,508
  504 AMPY=0.0
      AMUT=0.0
      AMVT=0.0
      DELET=0.0
      GO TO 503
  508 IF(AMX(K))504,504,98
   98 AMPY=(AMX(K)*V(K)*DT)/DY(J)
      GO TO 503
C     NO BOUNDARY CONDITIONS AT TOP INTERFACE
  304 IF((AMX(L).NE.0.) .AND. (JMR(KFIT(L),2).EQ.0)
     1    .AND. (J.EQ.J5-1)) GO TO 214
      IF( JMR(KFIT(L),2).EQ.0 ) GO TO 703
  214 IF(JMR(KFIT(K ),2).NE.0) GO TO 209
```

```
      DLTZ=DY(J+1)
      DLZ=FIOUT(K)
      FMT=.5
      VFR=P(K)
      IF((J.LT.JS-1).OR.(I.GT.ISR).OR.(AMX(K).NE.0.)) GO TO 216
      VFR=(GV+1.)*(-CO)/(GV-1.)
      P(K)=VFR
      GO TO 2166
  216 IF(ABS(V(L)).GT.ABS(P(K)))    VFR=V(L)
      IF((AMX(K).NE.0.).AND.(ABS(V(K)).GT.ABS(P(K)))) VFR=V(K)
      P(K)=VFR
 2166 VABOVE=V(L)+( VFR-V(L))*DY(J+1)/(DY(J+1)+2.*FIOUT(K))
      FIOUT(K)=ABS(VFR)*DT+FIOUT(K)
      IF(FIOUT(K).GE.DY(J)-1.E-7) P(KB)=P(K)
      IF((FIOUT(K).GE.DY(J)-1.E-7).AND.(JMR(KFIT(K+1),2).EQ.0))
     2           THETA(K+1)=THETA(K)
      IF(FIOUT(K).GE.DY(J)) FIOUT(KB)=FIOUT(K)-DY(J)
      FMT=(FIOUT(K)/(DLTZ+DLZ))**4*(1.-(DLZ/FIOUT(K))**4)*FMT
      IF(FMT.GT.1.) FMT=1.
      AMPY=-AMX(L)*FMT
      VFI=VABOVE**2+U(L)**2-AMX(K)/(AMX(K)-AMPY)*((V(K)-VABOVE)**2
     2           +(U(K)-U(L))**2)
      GO TO 503
  215 IF(JMR(KFIT(K),2).EQ.0) GO TO 504
  208 VABOVE=V(K)                                                    PH2 1510
      GO TO 212                                                      PH2 1520
  209 VABOVE=V(L)+(V(K)-V(L))*DY(J+1)/(DY(J+1)+DY(J))
  212 CONTINUE                                                       PH2 1540
      IF(VABOVE)701,703,700
  700 IF(AMX(K))703,703,704
  703 AMPY=0
      AMUT=0
      AMVT=0
      DELET=0
      GO TO 503
  704 KC=L
      KD=K
      JJ=J
      IF(((RHO(L).GT.RHO(K)).AND.(VABOVE.LT.0.)).OR.
     2   ((RHO(L).LT.RHO(K)).AND.(VABOVE.GE.0.)))
     3  GO TO 6140
      AMPY=TAU(I )*RHO(KD)*VABOVE*DT
      IF(V(KD)*V(KC).LT.0.) AMPY=0.
      GO TO 6150
 6140 AMPY= TAU(I)/3.*(RHO(L)*V(L)+RHO(K)*V(K)
     1+VABOVE*SQRT(RHO(K)*RHO(L)))*DT
      IF(AMPY*VABOVE.LT.0.) AMPY=0.
 6150 AVW=.5*(1.+RHO(KC)/RHO(KD))
      VABOVE=AVW*V(KD)+(1.-AVW)*V(KC)
      GO TO 503
  701 IF(AMX(L))703,703,705
  705 KC=K
      KD=L
      JJ=J+1
      IF(((RHO(L).GT.RHO(K)).AND.(VABOVE.LT.0.)).OR.
     2   ((RHO(L).LT.RHO(K)).AND.(VABOVE.GE.0.)))
     3  GO TO 6140
      AMPY=TAU(I )*RHO(KD)*VABOVE*DT
      IF(V(KD)*V(KC).LT.0.) AMPY=0.
      GO TO 6150
C     RIGHT INTERFACE OF CELL CALCULATION
  503 GO TO(405,405,405,706,405,405,405,405,706,706,
     1405,707,405,707,707,405),KFLAG
C     REFLECT AT RIGHT CELL INTERFACE
  706 IF(U(K))708,708,710
```

```
  708 AMUR=0.0
      GO TO 709
  710 AMMP=(AMX(K)*X(I)*2.0*U(K))/(TAU(I)*PIDTS)
      IF(AMMP-AMX(K))712,712,711
  711 AMMP=AMX(K)
  712 AMUR=2.0*AMMP*U(K)
  709 AMMP=0.0
      AMVR=0.0
      DELER=0.0
      GO TO 716
C     TRANSMIT AT RIGHT CELL INTERFACE
  707 IF(U(K))713,713,714
  713 AMMP=0.0
      AMUR=0.0
      AMVR=0.0
      DELER=0.0
      GO TO 716
  714 IF(AMX(K))713,713,715
  715 AMMP=(2.0*AMX(K)*X(I)*U(K))/(TAU(I)*PIDTS)
      GO TO 716
  405 IF(JMR(KFIT(K+1),2))411,411,409
  409 IF(AMX(K))410,410,407                                          PH2 1600
  410 URR=U(K+1)                                                     PH2 1610
      GO TO 408                                                      PH2 1620
  411 IF(JMR(KFIT(K),2).EQ.1) GO TO 406
  403 URR=0.0                                                        PH2 1640
      GO TO 408                                                      PH2 1650
  406 CONTINUE
      DLTZ= DX(I+1)
      DLZ= CAP(K+1)
      UFR=THETA(K+1)
      IF(ABS(U(K)).GT.ABS(THETA(K+1)))   UFR=U(K)
      IF(J.EQ.J5) UFR=2.*C0/(GV-1.)
      IF((AMX(K+1).NE.0.).AND.(ABS(U(K+1)).GT.ABS(THETA(K+1))))
     2           UFR=U(K+1)
      THETA(K+1)=UFR
      URR=U(K)+(UFR        -U(K))*DX(I)/(DX(I)+CAP(K+1))
      CAP(K+1)= ABS(UFR)*DT+CAP(K+1)
      IF(CAP(K+1).GE.DX(I+1)-1.E-7)THETA(K+2)=THETA(K+1)
      IF((CAP(K+1).GE.DX(I+1)-1.E-7).AND.(JMR(KFIT(KB+1),2).EQ.0))
     2           P(KB+1)=P(K+1)
      IF(CAP(K+1).GT.DX(I+1)) CAP(K+2)=CAP(K+1)-DX(I+1)
      FMT=(CAP(K+1)/(DLTZ+DLZ))**4*(1.-(DLZ/CAP(K+1))**4)
       FMT=.5*FMT
      IF(FMT.GT.1.)FMT=1.
      AMMP=AMX(K)*FMT
      UFI=URR**2+V(K)**2-AMX(K+1)/(AMX(K+1)+AMMP)*((U(K+1)-URR)**2
     2           +(V(K+1)-V(K))**2)
      GO TO 716
  407 URR=U(K)+(U(K+1)-U(K))*DX(I+1) /(DX(I)+DX(I+1))
  408 CONTINUE                                                       PH2 1700
C     NO BOUNDARY CONDITIONS AT RIGHT INTERFACE
      IF(URR)718,719,717
  717 IF(AMX(K))719,719,720
  720 KC=K+1
      KD=K
      GO TO 730
 6100 CONTINUE
      XB=X(I)-DX(I)/2.
      XBP=X(I+1)-DX(I+1)/2.
      AMMP =((RHO(K)*XB   *U(K)+RHO(K+1)*XBP    *U(K+1))
     1    +URR*X(I)*SQRT(RHO(K)*RHO(K+1)))*2./PIDTS*.33333*DY(J)
      IF(AMMP*URR.LT.0.) AMMP=0.
 6110 AUW=.5*(1.+RHO(KC) /RHO(KD))
      IF(AUW.GT.1.) AUW=1.
```

```
      URR=AUW*U(KD)+(1.-AUW)*U(KC)
      IF (U(K).NE.0.) GO TO 716
      URR=0.
  719 AMMP=0.0
      AMUR=0.0
      AMVR=0.0
      UELER=0.0
      GO TO 716
  718 IF(AMX(K+1))719,719,721
  721 KC=K
      KD=K+1
  730 IF(((RHO(K).GT.RHO(K+1)).AND. (URR.GT.0.)) .OR.
     2    ((RHO(K).LT.RHO(K+1)).AND. (URR.LT.0.)))
     3 TEST=DONNER
      AMMP=RHO(KD)*X(I)*URR*2./PIDTS*DY(J)
      IF(U(KD)*U(KC).LT.0.) AMMP=0.
      GO TO 6110
  716 CONTINUE
      IF(JMR(KFIT(K  ),2).EQ.0) GO TO 7260
      IF(J.EQ.J5) GO TO 7160
      IF(JMR(KFIT(L),2).EQ.0) GO TO 7160
      VPLUS=V(LP)+(V(L)-V(LP))*DY(J+2)/(DY(J+2)+DY(J+1))
      IF(VPLUS) 7020,7010,7010
 7010 KC=LP
      KD=L
      JJ=J+1
      GO TO 7030
 7020 KC=L
      KD=LP
      JJ=J+2
 7030 IF(( RHO(LP).GT.RHO(L)).AND.(VPLUS.LE.0.)) .OR.
     2    ( RHO(LP).LT.RHO(L)).AND.(VPLUS.GE.0.)))
     3 GO TO 7040
      AMMPY=TAU(I )*RHO(KD)*VPLUS*DT
      IF(V(KD)*V(KC).LT.0.) AMMPY=0.
      GO TO 7050
 7040 CONTINUE
      AMMPY=TAU(I)/3.*(RHO(LP)*V(LP)+RHO(L)*V(L)
     1      +VPLUS*SQRT(RHO(L)*RHO(LP)))*DT
      IF(AMMPY*VPLUS.LT.0.) AMMPY=0.
 7050 CONTINUE
      IF(JMR(KFIT(LP),2).EQ.0) AMMPY=0.
      IF( (J.EQ.J5-1).AND.(I.LE.ISR) ) AMMPY =-SOLID(IS+14  )
      IF( (J.EQ.J5-1).AND.(I.GT.ISR) ) AMMPY =0.
      UPS=U(L)+(U(L+1)-U(L))*DX(I)/(DX(I)+DX(I+1))
      IF(UPS)  7070,7065,7065
 7065 KD=L
      KC=L+1
      GO TO 7080
 7070 KC=L
      KD=L+1
 7080 IF (((RHO(L).GT.RHO(L+1)).AND.  (UPS.GT.0.)).OR.
     2        ((RHO(L).LT.RHO(L+1)).AND.(UPS.LT.0.)))
     3 TEST=DONNER
      AMMMP = RHO(KD)*X(I)*UPS*2./ PIDTS*DY(J)
      IF(U(KD)*U(KC).LT.0.)  AMMMP=0.
      GO TO 7095
 7090 CONTINUE
      XB=X(I)-DX(I)/2.
      XBP=X(I+1)-DX(I+1)/2.
      AMMMP= (RHO(L)*XB*U(L)+RHO(L+1)*XBP*U(L+1)
     1      +UPS*X(I)*SQRT(RHO(L)*RHO(L+1)))*2./PIDTS*.33333*DY(J+1)
      IF(AMMMP*UPS.LT.0.) AMMMP=0.
 7095 CONTINUE
      IF(JMR(KFIT(L+1),2).EQ.1)GO TO 7060
```

```
      IF(AMX(L+1).EQ.0.)       UFR =1.5*U(L)
      IF(ABS(THETA(L+1)).LT.ABS(U(L)))       UFR= U(L)
      ULTZ=UX(I+1)
      ULZ=CAP(L+1)
      CAPLP=CAP(L+1)+ABS(UFR)*DT
      FMT=(CAPLP/(ULTZ+ULZ))**4*(1.-(ULZ/CAPLP)**4)
       FMT=.5*FMT
      AMMMP=AMX(L)*(AMIN1(FMT,1.))
 7060 CONTINUE
      IF((GAMC(J+1)-AMMPY+AMX(L)*.5).GE.(AMMMP-AMPY)) GO TO 7160
      WSA =(GAMC(J+1)-AMMPY+AMX(L)*.5)/(AMMMP-AMPY)
      AMPY=AMPY*WSA
 7160 CONTINUE
      IF(JMR(KFIT(K+1),2).EQ.0) GO TO 7260
      AMMPY=AMPY
      IF((J.EQ.J5) .AND.(I.LE.ISR)) AMMPY=-SOLID(IS+14)
      IF((J.EQ.J5) .AND.(I.GT.ISR)) AMMPY=0.
      IF(GAMC(J)-AMMPY+AMX(K)*.5.GT.AMMP-AMMY) GO TO 7260
      AMMP = GAMC(J)-AMMPY+AMMY+AMX(K)*.5
      IF(AMMP.LT.0.) AMMP =0.
 7260 CONTINUE
      FLO=FLOUT(K)-(DY(J)-1.E-7)
  309 IF(AMPY)8834,8831,8833                                          PH2 3390
 8833 IF(JHIGH-J)9901,318,8835
 8835 IF(JMR(KFIT(K),2).EQ.1) GO TO 8837
      KM=K-IMAX
      IF(JMR(KFIT(KM ),2).EQ.0) GO TO 8838
      IF(FLO.LT.0.) GO TO 8837
      CALL MFST(KFIT(K),2)
      GO TO 318
 8837  IF( TAU(I  )*DY(J  )/  AMPY .LT.Z(138) ).GO TO 318
                                                                     PH2 3440
 8838 AMPY=0.0                                                       PH2 3450
      GO TO 8831
 8834 IF(J-JLOW)9902,325,8839
 8839 KP=K+IMAX
      IF(J.EQ.JHIGH) GO TO 8840
      IF(JMR(KFIT(K  ),2).EQ.1) GO TO 8840
      IF(JMR(KFIT(KP ),2).EQ.0) GO TO 8841
      IF(FLO.LT.0.) GO TO 8840
      CALL MFST(KFIT(K),2)
      GO TO 325
 8840  IF( TAU(I  )*DY(J+1)/(-AMPY).LT.Z(138) ) GO TO 325
                                                                     PH2 3490
 8841 AMPY=0.0                                                       PH2 3500
      GO TO 8831                                                     PH2 3510
  318 UELM=GAMC(J)+AMMY-AMPY
  322 IF(J-JHIGH)324,323,324                                         PH2 3530
  323 WS=U(K)**2+V(K)**2                                             PH2 3540
      ETH=ETH-AMPY*(AIX(K)+WS/2.0)                                   PH2 3550
      IF(AMPY/(TAU(I)*DY(J))-TOZONE)324,324,6900                     PH2 3560
 6900 REZ=1.0
  324 GO TO (6901,6901,326,6901,6901,6901,6901,326,326,
     16901,6901,6901,6901,6901,6901,6901),KFLAG
 6901 AMUT=AMPY*U(K)                                                 PH2 3580
      AMVT=AMPY*V(K)                                                 PH2 3590
      GO TO 326                                                      PH2 3600
  325 CONTINUE
 8831 GO TO(6902,6902,6903,6902,6902,6902,6902,6903,6903,
     16902,6902,6902,6902,6902,6902,6902),KFLAG
 6902 AMUT=AMPY*U(L)
      AMVT =AMPY*VABOVE
      IF(ABS(AMVT).GT.ABS(AMX(L)*V(L))) AMVT=SIGN((AMX(L)*V(L)),AMVT)
 6903 UELM=GAMC(J)-AMPY+AMMY
  326 IF(AMPY)327,328,328                                            PH2 3640
  327 DELET=AIX(L)+(U(L)**2+V(L)**2)/2.0                             PH2 3650
      IF( (I.GT.ISR) .OR.  (J.LT.J5) ) GO TO 3327
```

```
      DELET=HVB+HCB+SOLID(IS+15)**2/2.
      AMUT=0.
      AMVT=AMPY*SOLID(IS+15)
      ETH=ETH-AMPY*(HVB+HCB+SOLID(IS+15)**2/2.)
      GO TO 333
 3327 CONTINUE
      AMAS=RHO(K)/RHO(L)
      AMW= 0.63 + 0.235*AMAS
      IF(AMAS.GE..3)
     I AMW=.25+1.5*AMAS
      IF(AMW.GE.1.) AMW=1.
      DEKTT=AIX(K)+(U(L)**2+V(K)**2) /2.
      DELET=AMW*DELET+(1.-AMW)*DEKTT
      IF(JMR(KFIT(K),2).NE.1) DELET=HVB+HCB-HCP       +VF1/2.
      GO TO 333                                                    PH2 3660
  328 IF(AMMY)329,330,330                                          PH2 3670
  329 DELET=DELEB                                                  PH2 3680
      GO TO 333                                                    PH2 3690
  330 IF(GAMC(J))331,332,332                                       PH2 3700
  331 DELET=SIGC(J)                                                PH2 3710
      GO TO 333                                                    PH2 3720
  332 DELET=AIX(K)+(U(K)**2+V(K)**2)/2.0                           PH2 3730
  333 SIGMU=FLEFT(J)+AMMU-AMUT                                     PH2 3740
      SIGMV=YAMC(J)+AMMV-AMVT                                      PH2 3750
      DELEK=GAMC(J)*SIGC(J)+AMMY*DELEB-AMPY*DELET                  PH2 3760
      FLO=CAP(K+1)-(DX(I+1)-I.E-7)
  509 IF(AMMP)8843,518,8844                                        PH2 3770
 8844 IF(I.EQ.IMAX) GO TO 518
      IF(JMR(KFIT(K),2).NE.1) GO TO 8847
      IF(JMR(KFIT(K+1),2).EQ.I) GO TO 8846
      IF(FLO.LT.0.) GO TO 8846
      CALL MFST(KFIT(K+I),2)
      GO TO 518
 8846 GO TO 518
 8847 AMMP=0.0                                                     PH2 3810
      GO TO 518                                                    PH2 3820
 8843 IF(I.EQ.II+I) GO TO 512
      IF(JMR(KFIT(K+1),2).NE.1) GO TO 8850
      IF(JMR(KFIT(K  ),2).EQ.1) GO TO 8849
      IF(FLO.LT.0.) GO TO 8849
      CALL MFST(KFIT(K),2)
      GO TO 512
 8849  IF( TAU(I+I)*DY(J  )/(-AMMP).LT.Z(138) ) GO TO 512
 8850 AMMP=0.0                                                     PH2 3860
      GO TO 518                                                    PH2 3870
  512 DELM=DELM-AMMP+AMX(K)                                        PH2 3880
  513 CONTINUE                                                     PH2 3890
  514 CONTINUE                                                     PH2 3900
 8828 AMUR=AMMP*U(K+I)                                             PH2 3910
      AMVR=AMMP*V(K+I)                                             PH2 3920
      GO TO 525                                                    PH2 3930
  518 DELM=DELM-AMMP+AMX'K)                                        PH2 3940
  521 CONTINUE                                                     PH2 3950
  522 GO TO (524,524,524,524,524,524,524,524,524,
     I524,524,523,524,523,523,524),KFLAG
  523 WS=U(K)**2+V(K)**2                                           PH2 3970
      ETH=ETH-AMMP*(AIX(K)+WS/2.0)                                 PH2 3980
  524 AMUR = AMMP*URR
      IF(ABS(AMUR).GT.ABS(AMX(K)*U(K))) AMUR=SIGN((AMX(K)*U(K)),AMUR)
      AMVR=AMMP*V(K)                                               PH2 4020
  525 SIGMU=SIGMU-AMUR                                             PH2 4030
      SIGMV=SIGMV-AMVR                                             PH2 4040
  526 TIC=0.0                                                      PH2 4050
  531 IF(AMMP)532,533,534
  532 DELEK= AIX(K+1)+(U(K+1)**2+V(K+1)**2)/2.
```

```
      GO TO 535
  533 DELER=0.
      GO TO 535
  534 DELER= AIX(K)+(U(K)**2+V(K)**2) /2.
      AMAS = RHO(K+1)/RHO(K)
      AMW = 0.63+0.233*AMAS
      IF(AMAS.GE..3)
     1 AMW=.25+1.5*AMAS
      IF(AMW.GE.1.) AMW=1.
      DELTT=AIX(K+1)+(U(K+1)**2+V(K  )**2)/2.
      DELER=AMW*DELER+(1.-AMW)*DELTT
      IF(JMR(KF1T(K+1),2).NE.1)DELER=HVB+HCB-HCP+UF1/2.
  535 DELEK= DELEK-AMMP*DELER
      WS= AIX(K)+(U(K)**2+V(K)**2)/2.
  538 ETH=ETH+FSR+FSB
  540 ENK=AMX(K)*WS+DELEK+FSB+FSR
  541 U(K)=(SIGMU+AMX(K)*U(K))/DELM                                    PH2 4300
  601 V(K)=(SIGMV+AMX(K)*V(K))/DELM                                    PH2 4310
  603 WS=U(K)**2+V(K)**2                                               PH2 4400
  542 AIX(K)=ENK/DELM-WS/2.0                                           PH2 4410
  543 AMX(K)=DELM                                                      PH2 4420
      RHO(K)=AMX(K)/(DY(J)*TAU(1))
      IF(AMX(K).G T.0.) GO TO 544
       AIX(K)=0 .
      U(K)=0.0                                                         PH2 4450
      V(K)=0.0                                                         PH2 4460
      P(K)=0.0                                                         PH2 4470
      RHO(K)=0.
  544 GAMC(J)=AMMP                                                     PH2 4480
      FLEFT(J)=AMUR                                                    PH2 4490
      YAMC(J)=AMVR                                                     PH2 4500
      SIGC(J)=DELER                                                    PH2 4510
  545 AMMY=AMPY                                                        PH2 4520
      AMMU=AMUT                                                        PH2 4530
      AMMV=AMVT                                                        PH2 4540
      DELER=DELET                                                      PH2 4550
  702 CONTINUE
      GO TO (546,546,549,546,546,546,546,549,549,546,546,
     1546,546,546,546,546),KFLAG
  546 K=K+1MAX                                                         PH2 4560
      LL=K-1MAX
  549 CONTINUE
  547 CONTINUE                                                         PH2 4640
 6801 CONTINUE                                                         PH2 4720
 6802 GO TO 548                                                        PH2 4730
 9901 S1=9.8833
      GO TO 9999
 9902 S1=9.8834
 9999 CALL EDIT
  548 SUM=0.0                                                          PH2 4970
      DO 650 I=1,IMAX
      DO 650 J=1,JMAX
      K=(J-1)*1MAX+1+1
      IF((JMR(KF1T(K),2).EQ.2).AND.(AMX(K).GT.0.)) GO TO 610
      GO TO 645
  610 L=K+1MAX
      CALL MFST(KF1T(K),1)
  645 SV=1./RHO(K)
      IF(JMR(KF1T(K),2).NE.0)
     1CALL ES(SV,A1X(K),THETA(K),P(K),CAP(K),GG)
  650 CONTINUE
 8001 RETURN                                                           PH2 5260
      END                                                              PH2 5270
```

```
01    FOR  FLAG, FLAG/FJ
      SUBROUTINE FLAG(KFLAG,JLOW,JHIGH)
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),    AIX(1200),    P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200),  CAP(1200),    KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),     X(53),      XX(54),     DY(100),    Y(100),     YY(101),
     5TAU(15),    AMK(15),    PR(15),     QK(15),     Z(150),     IZ(150),
     6TAU(52),    PL(200),    PR(200),    UL(200),    UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON           Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON           AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON           BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON           DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON           P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON           PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON           RR,SIG,GOOOFL,SWITCH ,TABLM,TAU
      COMMON           TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON           UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON           VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON           VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON           WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON           XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON           I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON           IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON           JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON           L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON           ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON           NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON           FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                E   Q   U   I   V   A   L   E   N   C   E
C
     0EQUIVALENCE      (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
     0EQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
     1(Z(103),SVS),    (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFE),  (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
```

```
     3(Z(111),EZERO),   (Z(112),PW),     (Z(113),CAPS),    (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCR),    (Z(117),ISR),     (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),    (Z(121),IH),      (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),     (Z(125),JC),      (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),    (Z(129),HH),      (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),     (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                       (Z(138),SVMAX),
     8(Z(139),FRCDTC)
     0EQUIVALENCE       (Z(140),VAPE),   (Z(141),RADE),    (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),     (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),   (Z(149),DTUF),    (Z(150),E11)
C
     0EQUIVALENCE       (XX(2),X(1)),    (UR,UL,FLEFT),    (UR(100),YAMC),
     1(PR(100),SIGC),   (PR,PL,GAMC),    (DKE,THETA),      (UR,TAU),
     2(UR(16),AMK),     (UR(31),PK),     (UR(46),QK),      (YY(2),Y(1))
C
C
C                  C       O       M       M       O       N
C     TEST RIGHT BOUNDARY.
      IF(I.EQ.I1+1) GO TO 20
      IF(1.EQ.12) GO TO 40
C     TEST LEFT BOUNDARY.
      IF(I.EQ.IMAX) GO TO 60
      IF(1.LT.12) GO TO 40
      KFLAG=1
      IF(J.EQ.JLOW)KFLAG=5
      IF(J.EQ.JHIGH)KFLAG=7
      RETURN
   20 KFLAG=2
      IF(J.EQ.JLOW)KFLAG=11
      IF(J.EQ.JHIGH)KFLAG=8
      RETURN
   40 KFLAG=1
      IF(J.EQ.JLOW)KFLAG=5
      IF(J.EQ.JHIGH)KFLAG=3
      IF( (1.EQ.12).AND.(12.EQ.IMAX) ) GO TO 70
      RETURN
   60 KFLAG=12
      IF(J.EQ.JHIGH)KFLAG=14
   65 IF(J.EQ.JLOW)KFLAG=10
      RETURN
   70 KFLAG=12
      IF(J.EQ.JHIGH) KFLAG=9
      GO TO 65
      END
```

```
01    FOR  DJLOW, DJLOW/FJ
      SUBROUTINE DJLOW(JLOW,JHIGH)
C                 D  I  M  L  N  S  I  O  N
C
                        DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4UX(52),    X(53),     XX(54),     DY(100),    Y(100),    YY(101),
     5TAB(15),   AMK(15),   PK(15),     QK(15),     Z(150),    IZ(150),
     6TAU(52),   PL(200),   PR(200),    UL(200),    UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON          Z       ,XX      ,UK      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,GOOOFL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                 E  Q  U  I  V  A  L  E  N  C  E
C
     0EQUIVALENCE      (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),KSTOP),    (Z(73),SHELL),    (Z(74),RBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),WISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
      0EQUIVALENCE     (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
```

```
      EQUIVALENCE       (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
     1                  (Z(103),SVS),                       (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),    (Z(109),ALCO),
     3(Z(115),COE),     (Z(116),SCH),     (Z(117),ISR),     (Z(118),SCOR),
     4(Z(120),DTH),     (Z(121),IH),      (Z(122),JH),      (Z(123),DTC),
     5(Z(124),IC),      (Z(125),JC),
     6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                        (Z(138),SVMAX),
     8(Z(139),FRCUTC)
      EQUIVALENCE       (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),    (Z(149),DTUF),    (Z(150),EII)
C
      EQUIVALENCE       (XX(2),X(1)),     (UR,UL,FLEFT),    (UR(100),YAMC),
     1(PR(100),SIGC),   (PK,PL,GAMC),     (UKE,THETA),      (UR,TAB),
     2(UR(16),AMK),     (UR(31),PK),      (UR(46),QK),      (YY(2),Y(1))
C
C
C                  C       O       M       M       O       N
C
      IF(I.LE.I2) GO TO 20
      JLOW=1
      JHIGH=JMAX
      GO TO 100
   20 JLOW=1
      JHIGH=J5
  100 RETURN
      END
```

```
      FOR  LIBEX, LIBEX/FJ
      SUBROUTINE LIBEX(TAU,E,THA,P,ZBAR,GG)
      COMMON Z(90)
      EQUIVALENCE (Z(90),S1)
C*****PLACE DATA STATEMENTS PRODUCED BY PROGRAM GEST HERE  ******
      DATA TAUM,EM,TAUZ,EZ,V1,VZ/
     1 5.000E+10, 1.585E+12, 5.000E-02, 1.585E+09, 7.980E+00, 1.126E+03/
      DATA TAUZ,ELZ,S,T,PHI/
     1 -1.301E+0,  9.2,        2.000E+0,  8.000E+0,  5.244E+9/
      DATA NN,MM,I1,I2,I3,I4,I5,I6,I7,I8/
     1 25, 25,  1,  1,  1,  1,  1,  1,  0,  0/
      DIMENSION ZB(25,25),EILN(25,25)
      EQUIVALENCE (ZB,Z81), (EILN,EILN1)
      COMMON/EST/ZB 1(54)
      DATA ZB 1/
     1 2.200E-10, 3.912E-10, 6.957E-10, 1.237E-09, 2.200E-09, 3.912E-09,
     2 6.957E-09, 1.237E-08, 2.200E-08, 3.912E-08, 6.957E-08, 1.237E-07,
     3 2.200E-07, 3.911E-07, 6.955E-07, 1.236E-06, 2.197E-06, 3.904E-06,
     4 6.930E-06, 1.229E-05, 2.173E-05, 3.828E-05, 6.694E-05, 1.156E-04,
     5 1.957E-04, 3.911E-08, 6.956E-08, 1.237E-07, 2.200E-07, 3.911E-07,
     6 6.955E-07, 1.237E-06, 2.198E-06, 3.907E-06, 6.941E-06, 1.232E-05,
     7 2.184E-05, 3.863E-05, 6.803E-05, 1.189E-04, 2.054E-04, 3.475E-04,
     8 5.694E-04, 9.132E-04, 1.382E-03, 1.984E-03, 2.722E-03, 3.553E-03,
     9 4.455E-03, 5.399E-03, 2.001E-06, 3.563E-06, 6.333E-06, 1.125E-05/
      COMMON/EST/ZB 2(54)
      DATA ZB 2/
     1 1.997E-05, 3.542E-05, 6.265E-05, 1.104E-04, 1.932E-04, 3.342E-04,
     2 5.669E-04, 9.331E-04, 1.499E-03, 2.279E-03, 3.284E-03, 4.485E-03,
     3 5.898E-03, 7.394E-03, 8.953E-03, 1.054E-02, 1.217E-02, 1.375E-02,
     4 1.529E-02, 1.679E-02, 1.823E-02, 4.031E-05, 7.149E-05, 1.263E-04,
     5 2.223E-04, 3.879E-04, 6.677E-04, 1.124E-03, 1.847E-03, 2.903E-03,
     6 4.337E-03, 6.138E-03, 8.283E-03, 1.064E-02, 1.312E-02, 1.566E-02,
     7 1.820E-02, 2.075E-02, 2.318E-02, 2.552E-02, 2.776E-02, 2.989E-02,
     8 3.192E-02, 3.384E-02, 3.567E-02, 3.739E-02, 3.950E-04, 6.918E-04,
     9 1.189E-03, 1.996E-03, 3.264E-03, 5.096E-03, 7.557E-03, 1.060E-02/
      COMMON/EST/ZB 3(54)
      DATA ZB 3/
     1 1.416E-02, 1.801E-02, 2.200E-02, 2.601E-02, 2.995E-02, 3.382E-02,
     2 3.747E-02, 4.093E-02, 4.419E-02, 4.725E-02, 5.013E-02, 5.283E-02,
     3 5.535E-02, 5.772E-02, 5.994E-02, 6.203E-02, 6.399E-02, 2.214E-03,
     4 3.697E-03, 5.987E-03, 9.230E-03, 1.348E-02, 1.861E-02, 2.446E-02,
     5 3.061E-02, 3.685E-02, 4.298E-02, 4.887E-02, 5.446E-02, 5.981E-02,
     6 6.471E-02, 6.927E-02, 7.349E-02, 7.741E-02, 8.103E-02, 8.439E-02,
     7 8.751E-02, 9.041E-02, 9.310E-02, 9.561E-02, 9.795E-02, 1.001E-01,
     8 7.936E-03, 1.251E-02, 1.867E-02, 2.629E-02, 3.501E-02, 4.446E-02,
     9 5.399E-02, 6.331E-02, 7.220E-02, 8.052E-02, 8.823E-02, 9.533E-02/
      COMMON/EST/ZB 4(54)
      DATA ZB 4/
     1 1.018E-01, 1.079E-01, 1.134E-01, 1.184E-01, 1.230E-01, 1.272E-01,
     2 1.311E-01, 1.346E-01, 1.379E-01, 1.410E-01, 1.438E-01, 1.464E-01,
     3 1.489E-01, 2.062E-02, 3.056E-02, 4.261E-02, 5.613E-02, 7.047E-02,
     4 8.465E-02, 9.826E-02, 1.110E-01, 1.227E-01, 1.334E-01, 1.431E-01,
     5 1.518E-01, 1.597E-01, 1.668E-01, 1.733E-01, 1.792E-01, 1.845E-01,
     6 1.894E-01, 1.938E-01, 1.979E-01, 2.016E-01, 2.051E-01, 2.083E-01,
     7 2.112E-01, 2.140E-01, 4.294E-02, 6.053E-02, 8.040E-02, 1.013E-01,
     8 1.223E-01, 1.421E-01, 1.605E-01, 1.772E-01, 1.922E-01, 2.057E-01,
     9 2.177E-01, 2.284E-01, 2.380E-01, 2.465E-01, 2.542E-01, 2.612E-01/
      COMMON/EST/ZB 5(54)
      DATA ZB 5/
     1 2.674E-01, 2.731E-01, 2.783E-01, 2.830E-01, 2.873E-01, 2.913E-01,
     2 2.950E-01, 2.983E-01, 3.015E-01, 7.700E-02, 1.047E-01, 1.346E-01,
     3 1.647E-01, 1.936E-01, 2.207E-01, 2.450E-01, 2.667E-01, 2.859E-01,
     4 3.029E-01, 3.178E-01, 3.310E-01, 3.426E-01, 3.532E-01, 3.624E-01,
     5 3.708E-01, 3.782E-01, 3.850E-01, 3.911E-01, 3.966E-01, 4.016E-01,
     6 4.061E-01, 4.103E-01, 4.146E-01, 4.182E-01, 1.244E-01, 1.652E-01,
```

```
     7 2.078E-01, 2.497E-01, 2.891E-01, 3.250E-01, 3.570E-01, 3.850E-01,
     8 4.100E-01, 4.316E-01, 4.505E-01, 4.671E-01, 4.817E-01, 4.948E-01,
     9 5.054E-01, 5.145E-01, 5.226E-01, 5.299E-01, 5.368E-01, 5.427E-01/
       COMMON/EST/ZB 6(54)
       DATA ZB 6/
     1 5.481E-01, 5.530E-01, 5.575E-01, 5.616E-01, 5.654E-01, 1.863E-01,
     2 2.434E-01, 3.020E-01, 3.588E-01, 4.117E-01, 4.595E-01, 5.017E-01,
     3 5.345E-01, 5.624E-01, 5.855E-01, 6.052E-01, 6.218E-01, 6.370E-01,
     4 6.499E-01, 6.613E-01, 6.715E-01, 6.806E-01, 6.887E-01, 6.960E-01,
     5 7.026E-01, 7.087E-01, 7.142E-01, 7.192E-01, 7.239E-01, 7.281E-01,
     6 2.629E-01, 3.396E-01, 4.174E-01, 4.923E-01, 5.592E-01, 6.139E-01,
     7 6.593E-01, 6.960E-01, 7.272E-01, 7.534E-01, 7.758E-01, 7.950E-01,
     8 8.117E-01, 8.262E-01, 8.390E-01, 8.504E-01, 8.605E-01, 8.695E-01,
     9 8.777E-01, 8.851E-01, 8.918E-01, 8.979E-01, 9.035E-01, 9.087E-01/
       COMMON/EST/ZB 7(54)
       DATA ZB 7/
     1 9.135E-01, 3.533E-01, 4.511E-01, 5.555E-01, 6.501E-01, 7.268E-01,
     2 7.895E-01, 8.404E-01, 8.818E-01, 9.168E-01, 9.463E-01, 9.714E-01,
     3 9.929E-01, 1.012E 00, 1.020E 00, 1.042E 00, 1.055E 00, 1.066E 00,
     4 1.076E 00, 1.085E 00, 1.093E 00, 1.101E 00, 1.108E 00, 1.114E 00,
     5 1.120E 00, 1.125E 00, 4.540E-01, 5.919E-01, 7.244E-01, 8.329E-01,
     6 9.206E-01, 9.915E-01, 1.049E 00, 1.096E 00, 1.135E 00, 1.168E 00,
     7 1.196E 00, 1.220E 00, 1.241E 00, 1.259E 00, 1.275E 00, 1.289E 00,
     8 1.302E 00, 1.313E 00, 1.323E 00, 1.332E 00, 1.340E 00, 1.348E 00,
     9 1.355E 00, 1.361E 00, 1.367E 00, 6.232E-01, 7.683E-01, 9.209E-01/
       COMMON/EST/ZB 8(47)
       DATA ZB 8/
     1 1.045E 00, 1.144E 00, 1.224E 00, 1.289E 00, 1.341E 00, 1.386E 00,
     2 1.422E 00, 1.453E 00, 1.480E 00, 1.504E 00, 1.525E 00, 1.544E 00,
     3 1.560E 00, 1.575E 00, 1.588E 00, 1.600E 00, 1.611E 00, 1.619E 00,
     4 1.628E 00, 1.636E 00, 1.644E 00, 1.650E 00, 8.692E-01, 9.739E-01,
     5 1.149E 00, 1.290E 00, 1.402E 00, 1.492E 00, 1.569E 00, 1.633E 00,
     6 1.686E 00, 1.730E 00, 1.768E 00, 1.799E 00, 1.827E 00, 1.851E 00,
     7 1.872E 00, 1.890E 00, 1.907E 00, 1.922E 00, 1.935E 00, 1.947E 00,
     8 1.958E 00, 1.968E 00, 1.977E 00, 1.985E 00, 1.993E 00/
       COMMON/EST/ZB 9(29)
       DATA ZB 9/
     5              9.721E-1, 1.216E+0, 1.415E+0, 1.580E+0, 1.718E+0,
     6  1.829E+0, 1.918E+0, 1.991E+0, 2.051E+0, 2.100E+0, 2.143E+0,
     7  2.180E+0, 2.211E+0, 2.239E+0, 2.263E+0, 2.284E+0, 2.303E+0,
     8  2.320E+0, 2.335E+0, 2.348E+0, 2.361E+0, 2.372E+0, 2.382E+0,
     9  2.391E+0, 2.401E+0, 1.217E+0, 1.497E+0, 1.743E+0, 1.944E+0/
       COMMON/EST/ZB10(54)
       DATA ZB10/
     1  2.103E+0, 2.229E+0, 2.331E+0, 2.415E+0, 2.485E+0, 2.538E+0,
     2  2.584E+0, 2.623E+0, 2.656E+0, 2.685E+0, 2.711E+0, 2.733E+0,
     3  2.754E+0, 2.772E+0, 2.788E+0, 2.803E+0, 2.817E+0, 2.828E+0,
     4  2.839E+0, 2.850E+0, 2.859E+0, 1.505E+0, 1.854E+0, 2.143E+0,
     5  2.373E+0, 2.550E+0, 2.681E+0, 2.786E+0, 2.872E+0, 2.943E+0,
     6  3.003E+0, 3.054E+0, 3.097E+0, 3.135E+0, 3.168E+0, 3.197E+0,
     7  3.223E+0, 3.246E+0, 3.266E+0, 3.285E+0, 3.301E+0, 3.317E+0,
     8  3.331E+0, 3.343E+0, 3.355E+0, 3.366E+0, 1.870E+0, 2.278E+0,
     9  2.600E+0, 2.834E+0, 3.019E+0, 3.164E+0, 3.284E+0, 3.381E+0/
       COMMON/EST/ZB11(54)
       DATA ZB11/
     1  3.461E+0, 3.527E+0, 3.582E+0, 3.630E+0, 3.672E+0, 3.708E+0,
     2  3.739E+0, 3.768E+0, 3.793E+0, 3.815E+0, 3.836E+0, 3.854E+0,
     3  3.871E+0, 3.886E+0, 3.900E+0, 3.913E+0, 3.925E+0, 2.303E+0,
     4  2.746E+0, 3.082E+0, 3.344E+0, 3.548E+0, 3.706E+0, 3.834E+0,
     5  3.938E+0, 4.025E+0, 4.098E+0, 4.161E+0, 4.214E+0, 4.261E+0,
     6  4.301E+0, 4.337E+0, 4.369E+0, 4.397E+0, 4.422E+0, 4.445E+0,
     7  4.466E+0, 4.485E+0, 4.502E+0, 4.518E+0, 4.532E+0, 4.545E+0,
     8  2.780E+0, 3.256E+0, 3.627E+0, 3.909E+0, 4.130E+0, 4.307E+0,
     9  4.449E+0, 4.566E+0, 4.661E+0, 4.743E+0, 4.812E+0, 4.872E+0/
       COMMON/EST/ZB12(54)
```

```
      DATA ZB12/
     1  4.924E+0,  4.969E+0,  5.009E+0,  5.045E+0,  5.076E+0,  5.105E+0,
     2  5.130E+0,  5.153E+0,  5.174E+0,  5.194E+0,  5.211E+0,  5.228E+0,
     3  5.243E+0,  3.307E+0,  3.828E+0,  4.230E+0,  4.544E+0,  4.789E+0,
     4  4.986E+0,  5.145E+0,  5.274E+0,  5.383E+0,  5.474E+0,  5.536E+0,
     5  5.582E+0,  5.623E+0,  5.659E+0,  5.692E+0,  5.721E+0,  5.748E+0,
     6  5.772E+0,  5.794E+0,  5.814E+0,  5.833E+0,  5.850E+0,  5.866E+0,
     7  5.880E+0,  5.894E+0,  5.901E+0,  4.474E+0,  4.921E+0,  5.267E+0,
     8  5.526E+0,  5.658E+0,  5.767E+0,  5.859E+0,  5.939E+0,  6.007E+0,
     9  6.067E+0,  6.119E+0,  6.166E+0,  6.207E+0,  6.244E+0,  6.277E+0/
      COMMON/EST/ZB13( 9)
      DATA ZB13/
     1  6.306E+0,  6.334E+0,  6.358E+0,  6.381E+0,  6.402E+0,  6.419E+0,
     2  6.437E+0,  6.453E+0,  6.468E+0/
      COMMON/EST/EILN 1(54)
      DATA EILN 1/
    1-1.961E 01,-1.961E 01,-1.961E 01,-1.822E 01,-1.782E 01,-1.731E 01,
    2-1.672E 01,-1.614E 01,-1.555E 01,-1.498E 01,-1.440E 01,-1.383E 01,
    3-1.325E 01,-1.268E 01,-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,
    4-9.802E 00,-9.229E 00,-8.659E 00,-8.093E 00,-7.534E 00,-6.987E 00,
    5-6.461E 00,-1.499E 01,-1.440E 01,-1.383E 01,-1.325E 01,-1.268E 01,
    6-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,-9.800E 00,-9.227E 00,
    7-8.654E 00,-8.084E 00,-7.518E 00,-6.959E 00,-6.413E 00,-5.887E 00,
    8-5.393E 00,-4.921E 00,-4.507E 00,-4.145E 00,-3.829E 00,-3.562E 00,
    9-3.336E 00,-3.144E 00,-1.104E 01,-1.047E 01,-9.892E 00,-9.317E 00/
      COMMON/EST/EILN 2(54)
      DATA EILN 2/
    1-8.743E 00,-8.171E 00,-7.600E 00,-7.034E 00,-6.474E 00,-5.926E 00,
    2-5.398E 00,-4.899E 00,-4.425E 00,-4.006E 00,-3.641E 00,-3.329E 00,
    3-3.055E 00,-2.829E 00,-2.638E 00,-2.475E 00,-2.331E 00,-2.209E 00,
    4-2.103E 00,-2.009E 00,-1.927E 00,-8.041E 00,-7.468E 00,-6.899E 00,
    5-6.334E 00,-5.777E 00,-5.234E 00,-4.713E 00,-4.216E 00,-3.764E 00,
    6-3.363E 00,-3.016E 00,-2.716E 00,-2.466E 00,-2.256E 00,-2.079E 00,
    7-1.929E 00,-1.797E 00,-1.687E 00,-1.591E 00,-1.506E 00,-1.432E 00,
    8-1.367E 00,-1.308E 00,-1.256E 00,-1.209E 00,-5.759E 00,-5.199E 00,
    9-4.657E 00,-4.139E 00,-3.647E 00,-3.202E 00,-2.808E 00,-2.469E 00/
      COMMON/EST/EILN 3(54)
      DATA EILN 3/
    1-2.179E 00,-1.939E 00,-1.739E 00,-1.572E 00,-1.431E 00,-1.309E 00,
    2-1.207E 00,-1.118E 00,-1.042E 00,-9.745E-01,-9.154E-01,-8.630E-01,
    3-8.163E-01,-7.744E-01,-7.366E-01,-7.024E-01,-6.714E-01,-4.035E 00,
    4-3.523E 00,-3.040E 00,-2.608E 00,-2.229E 00,-1.906E 00,-1.633E 00,
    5-1.409E 00,-1.223E 00,-1.069E 00,-9.409E-01,-8.327E-01,-7.390E-01,
    6-6.601E-01,-5.921E-01,-5.329E-01,-4.810E-01,-4.352E-01,-3.946E-01,
    7-3.583E-01,-3.257E-01,-2.964E-01,-2.698E-01,-2.456E-01,-2.235E-01,
    8-2.759E 00,-2.303E 00,-1.903E 00,-1.561E 00,-1.275E 00,-1.035E 00,
    9-8.412E-01,-6.819E-01,-5.506E-01,-4.415E-01,-3.501E-01,-2.727E-01/
      COMMON/EST/EILN 4(54)
      DATA EILN 4/
    1-2.067E-01,-1.484E-01,-9.905E-02,-5.591E-02,-1.794E-02, 1.568E-02,
    2 4.563E-02, 7.246E-02, 9.660E-02, 1.184E-01, 1.383E-01, 1.564E-01,
    3 1.729E-01,-1.804E 00,-1.411E 00,-1.078E 00,-8.024E-01,-5.749E-01,
    4-3.915E-01,-2.424E-01,-1.206E-01,-2.026E-02, 6.316E-02, 1.332E-01,
    5 1.925E-01, 2.432E-01, 2.870E-01, 3.250E-01, 3.583E-01, 3.876E-01,
    6 4.136E-01, 4.368E-01, 4.576E-01, 4.764E-01, 4.934E-01, 5.088E-01,
    7 5.229E-01, 5.358E-01,-1.070E 00,-7.269E-01,-4.430E-01,-2.121E-01,
    8-2.386E-02, 1.265E-01, 2.481E-01, 3.471E-01, 4.286E-01, 4.962E-01,
    9 5.529E-01, 6.010E-01, 6.420E-01, 6.774E-01, 7.082E-01, 7.351E-01/
      COMMON/EST/EILN 5(54)
      DATA EILN 5/
    1 7.588E-01, 7.799E-01, 7.986E-01, 8.154E-01, 8.306E-01, 8.443E-01,
    2 8.568E-01, 8.682E-01, 8.786E-01,-4.863E-01,-1.788E-01, 7.220E-02,
    3 2.742E-01, 4.359E-01, 5.668E-01, 6.712E-01, 7.560E-01, 8.256E-01,
    4 8.832E-01, 9.314E-01, 9.722E-01, 1.006E 00, 1.037E 00, 1.063E 00,
    5 1.086E 00, 1.105E 00, 1.123E 00, 1.139E 00, 1.153E 00, 1.165E 00,
```

```
     6 1.177E 00, 1.187E 00, 1.197E 00, 1.206E 00,-6.935E-03, 2.768E-01,
     7 5.063E-01, 6.901E-01, 8.367E-01, 9.538E-01, 1.048E 00, 1.123E 00,
     8 1.186E 00, 1.238E 00, 1.280E 00, 1.317E 00, 1.347E 00, 1.374E 00,
     9 1.395E 00, 1.413E 00, 1.429E 00, 1.444E 00, 1.457E 00, 1.469E 00/
       COMMON/EST/EILN 6(54)
       DATA EILN 6/
     1 1.479E 00, 1.488E 00, 1.497E 00, 1.505E 00, 1.512E 00, 3.972E-01,
     2 6.645E-01, 8.802E-01, 1.053E 00, 1.190E 00, 1.300E 00, 1.388E 00,
     3 1.455E 00, 1.506E 00, 1.550E 00, 1.587E 00, 1.617E 00, 1.644E 00,
     4 1.668E 00, 1.688E 00, 1.706E 00, 1.722E 00, 1.736E 00, 1.748E 00,
     5 1.760E 00, 1.770E 00, 1.779E 00, 1.788E 00, 1.796E 00, 1.803E 00,
     6 7.419E-01, 9.976E-01, 1.204E 00, 1.369E 00, 1.500E 00, 1.603E 00,
     7 1.684E 00, 1.748E 00, 1.801E 00, 1.845E 00, 1.882E 00, 1.913E 00,
     8 1.939E 00, 1.962E 00, 1.982E 00, 2.000E 00, 2.015E 00, 2.029E 00,
     9 2.042E 00, 2.055E 00, 2.063E 00, 2.072E 00, 2.080E 00, 2.088E 00/
       COMMON/EST/EILN 7(54)
       DATA EILN 7/
     1 2.095E 00, 1.037E 00, 1.282E 00, 1.493E 00, 1.668E 00, 1.801E 00,
     2 1.904E 00, 1.985E 00, 2.048E 00, 2.100E 00, 2.143E 00, 2.179E 00,
     3 2.209E 00, 2.235E 00, 2.258E 00, 2.277E 00, 2.295E 00, 2.310E 00,
     4 2.323E 00, 2.33[illegible] 00, 2.346E 00, 2.356E 00, 2.365E 00, 2.373E 00,
     5 2.381E 00, 2.387E 00, 1.288E 00, 1.562E 00, 1.797E 00, 1.973E 00,
     6 2.106E 00, 2.207E 00, 2.286E 00, 2.349E 00, 2.400E 00, 2.442E 00,
     7 2.477E 00, 2.506E 00, 2.532E 00, 2.554E 00, 2.573E 00, 2.589E 00,
     8 2.604E 00, 2.617E 00, 2.629E 00, 2.640E 00, 2.649E 00, 2.658E 00,
     9 2.666E 00, 2.673E 00, 2.680E 00, 1.619E 00, 1.870E 00, 2.106E 00/
       COMMON/EST/EILN 8(47)
       DATA EILN 8/
     1 2.281E 00, 2.412E 00, 2.512E 00, 2.589E 00, 2.650E 00, 2.700E 00,
     2 2.741E 00, 2.774E 00, 2.803E 00, 2.828E 00, 2.850E 00, 2.869E 00,
     3 2.886E 00, 2.901E 00, 2.914E 00, 2.926E 00, 2.936E 00, 2.944E 00,
     4 2.953E 00, 2.961E 00, 2.968E 00, 2.974E 00, 2.029E 00, 2.183E 00,
     5 2.419E 00, 2.591E 00, 2.718E 00, 2.815E 00, 2.895E 00, 2.958E 00,
     6 3.008E 00, 3.049E 00, 3.082E 00, 3.110E 00, 3.134E 00, 3.154E 00,
     7 3.172E 00, 3.188E 00, 3.202E 00, 3.214E 00, 3.225E 00, 3.234E 00,
     8 3.243E 00, 3.251E 00, 3.258E 00, 3.265E 00, 3.271E 00/
       COMMON/EST/EILN 9(29)
       DATA EILN 9/
     5           2.180E+0, 2.501E+0, 2.732E+0, 2.906E+0, 3.038E+0,
     6  3.136E+0, 3.211E+0, 3.270E+0, 3.316E+0, 3.354E+0, 3.386E+0,
     7  3.412E+0, 3.435E+0, 3.455E+0, 3.472E+0, 3.487E+0, 3.500E+0,
     8  3.511E+0, 3.522E+0, 3.530E+0, 3.539E+0, 3.546E+0, 3.553E+0,
     9  3.559E+0, 3.565E+0, 2.504E+0, 2.820E+0, 3.061E+0, 3.232E+0/
       COMMON/EST/EILN10(54)
       DATA EILN10/
     1  3.356E+0, 3.447E+0, 3.519E+0, 3.575E+0, 3.620E+0, 3.654E+0,
     2  3.683E+0, 3.707E+0, 3.728E+0, 3.746E+0, 3.762E+0, 3.775E+0,
     3  3.788E+0, 3.799E+0, 3.808E+0, 3.817E+0, 3.826E+0, 3.833E+0,
     4  3.839E+0, 3.846E+0, 3.851E+0, 2.829E+0, 3.157E+0, 3.385E+0,
     5  3.547E+0, 3.662E+0, 3.744E+0, 3.807E+0, 3.858E+0, 3.900E+0,
     6  3.935E+0, 3.965E+0, 3.989E+0, 4.011E+0, 4.029E+0, 4.045E+0,
     7  4.060E+0, 4.072E+0, 4.083E+0, 4.093E+0, 4.103E+0, 4.111E+0,
     8  4.118E+0, 4.125E+0, 4.131E+0, 4.137E+0, 3.171E+0, 3.482E+0,
     9  3.693E+0, 3.836E+0, 3.945E+0, 4.027E+0, 4.093E+0, 4.145E+0/
       COMMON/EST/EILN11(54)
       DATA EILN11/
     1  4.188E+0, 4.222E+0, 4.251E+0, 4.275E+0, 4.296E+0, 4.315E+0,
     2  4.331E+0, 4.345E+0, 4.357E+0, 4.369E+0, 4.379E+0, 4.388E+0,
     3  4.396E+0, 4.403E+0, 4.410E+0, 4.417E+0, 4.422E+0, 3.500E+0,
     4  3.783E+0, 3.980E+0, 4.125E+0, 4.233E+0, 4.314E+0, 4.378E+0,
     5  4.429E+0, 4.471E+0, 4.506E+0, 4.535E+0, 4.560E+0, 4.581E+0,
     6  4.600E+0, 4.616E+0, 4.630E+0, 4.643E+0, 4.655E+0, 4.665E+0,
     7  4.674E+0, 4.682E+0, 4.690E+0, 4.697E+0, 4.703E+0, 4.709E+0,
     8  3.804E+0, 4.078E+0, 4.274E+0, 4.415E+0, 4.521E+0, 4.602E+0,
     9  4.667E+0, 4.718E+0, 4.759E+0, 4.794E+0, 4.823E+0, 4.848E+0/
```

```
      COMMON/EST/EILN12(54)
      DATA EILN12/
     1  4.870E+0,  4.888E+0,  4.905E+0,  4.919E+0,  4.932E+0,  4.943E+0,
     2  4.953E+0,  4.962E+0,  4.971E+0,  4.978E+0,  4.985E+0,  4.992E+0,
     3  4.997E+0,  4.106E+0,  4.375E+0,  4.567E+0,  4.709E+0,  4.814E+0,
     4  4.895E+0,  4.959E+0,  5.010E+0,  5.052E+0,  5.086E+0,  5.109E+0,
     5  5.127E+0,  5.143E+0,  5.158E+0,  5.171E+0,  5.183E+0,  5.194E+0,
     6  5.204E+0,  5.214E+0,  5.222E+0,  5.230E+0,  5.238E+0,  5.245E+0,
     7  5.251E+0,  5.257E+0,  4.411E+0,  4.678E+0,  4.869E+0,  5.007E+0,
     8  5.105E+0,  5.157E+0,  5.202E+0,  5.242E+0,  5.277E+0,  5.308E+0,
     9  5.335E+0,  5.359E+0,  5.380E+0,  5.399E+0,  5.416E+0,  5.432E+0/
      COMMON/EST/EILN13( 9)
      DATA EILN13/
     1  5.446E+0,  5.458E+0,  5.470E+0,  5.481E+0,  5.490E+0,  5.499E+0,
     2  5.507E+0,  5.515E+0,  5.522E+0/
      IF(E.NE.0.) GO TO 5
      THA = 1.E-3
      ZBAR=0.
      GO TO 950
    5 CONTINUE
      ALGT=ALOG10(TAU)
      ALGE=ALOG10(E)
      DLGT=ALGT-TAULZ
      DLGE=ALGE-ELZ
      AN=DLGT*S+1.
      AM=DLGE*T+1.
      IF (DLGT.LT.0.) AN=0.
      IF(DLGE.LT.0.) AM=0.
      N=IFIX(AN)
      M=IFIX(AM)
      IN=0
      EO=E
      IF(N.LE.0) GO TO 10
      IF(N.GE.NN) GO TO 20
      IF(M.LE.0) GO TO 800
      IF(M.GE.MM) GO TO 400
    8 CONTINUE
      DNLT=AN-AINT(AN)
      DMLE=AM-AINT(AM)
      ZBAR=ZB(N,M)+(ZB(N+1,M)-ZB(N,M))* DNLT
     1            +(ZB(N,M+1)-ZB(N,M))* DMLE
     2            +(ZB(N+1,M+1)+ZB(N,M)-ZB(N+1,M)-ZB(N,M+1))
     3            *(DNLT*DMLE)
      ALIN=EILN(N,M)+(EILN(N+1,M)-EILN(N,M))*DNLT
     1              +(EILN(N,M+1)-EILN(N,M))*DMLE
     3              *(DNLT*DMLE)
     2              +(EILN(N+1,M+1)+EILN(N,M)-EILN(N+1,M)-EILN(N,M+1))
      THA=(EO/PHI-EXP(ALIN))/(1.5*(1.+ZBAR   ))
      IF(IN.NE.0)GO TO (150,250,350,450,550,650,750,850),IN
      GO TO 950
   10 IF(M.LE.0) GO TO 100
      IF(M.GE.MM) GO TO 300
      GO TO 200
   20 IF(M.LE.0) GO TO 700
      IF(M.GE.MM) GO TO 500
      GO TO 600
  100 CONTINUE
      IF(I1.EQ.1) GO TO 9901
  150 CONTINUE
      RETURN
  200 CONTINUE
      IF(I2.EQ.1) GO TO 9902
  250 CONTINUE
      RETURN
  300 CONTINUE
```

```
      IF(I3.EQ.1) GO TO 9903
  350 CONTINUE
      RETURN
  400 CONTINUE
      IF(I4.EQ.1) GO TO 9904
  450 CONTINUE
      RETURN
  500 CONTINUE
      IF(I5.EQ.1) GO TO 9905
  550 CONTINUE
      RETURN
  600 CONTINUE
      IF(I6.EQ.1) GO TO 9906
  650 CONTINUE
      RETURN
  700 CONTINUE
      IF(I7.EQ.1) GO TO 9907
      IN = 7
      M = 1
      N = NN
      EQ=EZ
      GO TO 8
  750 THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * SQRT(TAUM/TAU)*EXP(V1*(THAP-THA) /
     1 (THA*THAP*2.))
      AIN=V1*ZBAR
      GO TO 900
  800 CONTINUE
      IF(I8.EQ.1) GO TO 9908
      IN = 8
      M = 1
      EQ=EZ
      GO TO 8
  850 THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * EXP(V1*( THAP - THA) /
     1(THA * THAP*2.))
      AIN=V1*ZBAR
  900 CONTINUE
      THA=(E/PHI-AIN)/(1.5*(1.+ZBAR))
  950 P=PHI*(1.+ZBAR    )*THA/TAU
      RETURN
 9901 S1=12.0100
      GO TO 9999
 9902 S1=12.0200
      GO TO 9999
 9903 S1=12.0300
      GO TO 9999
 9904 S1=12.0400
      GO TO 9999
 9905 S1=12.0500
      GO TO 9999
 9906 S1=12.0600
      GO TO 9999
 9907 S1=12.0700
      GO TO 9999
 9908 S1=12.0800
 9999 WRITE(6,1000)TAU,E,THA,P,ZBAR,GG,ALGT
 1000 FORMAT(1H1,12X,6HTAU     ,9X,6HE       ,9X,6HTHA     ,9X,6HP       ,9X,6HZ
     1BAR   ,9X,6HGG      ,9X,6HALGT   /7X,1P7E15.7)
      WRITE(6,1001)ALGE,DLGT,DLGE,AN,AM
 1001 FORMAT(1H0,12X,6HALGE    ,9X,6HDLGT    ,9X,6HDLGE    ,9X,6HAN      ,9X,6HA
     1M      /7X,1P5E15.7)
      WRITE(6,1002)N,M,NN,MM,S1
 1002 FORMAT(1H0,12X,6HN       ,9X,6HM       ,9X,6HNN      ,9X,6HMM      ,9X,6HS
     11      /7X,I9,3(6X,I9),1PE15.7)
```

```
      CALL EDIT
      END
```

```
$I     FOR  ES, ES/FJ
       SUBROUTINE ES(TAU,E,THA,P,ZB,G)
       COMMON // Z
C                  E  Q  U  I  V  A  L  E  N  C  E
C
      OEQUIVALENCE      (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),    (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIOY),      (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),     (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),     (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),    (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),     (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),      (Z(29),NPRI),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),      (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),    (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
      OEQUIVALENCE      (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),      (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),       (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),       (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),       (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),       (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),     (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),    (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),REZFCT),   (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),BBOUND),
     9(Z(75),TOZONE),   (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
      OEQUIVALENCE      (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),    (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),     (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),       (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),       (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),       (Z(99),S10)
C
      OEQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
     1(Z(103),SVS),     (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
     3(Z(111),EZERO),   (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCK),     (Z(117),ISR),     (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),     (Z(121),IH),      (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),     (Z(129),HH),      (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                        (Z(138),SVMAX),
     8(Z(139),FRCUTC)
      OEQUIVALENCE      (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),    (Z(149),DTUF),    (Z(150),EII)
       A= E-HVB-HCB+HCP
       TEMPA=5.E+6
       IF(A.LT.TEMPA) A=0.0
       CALL LIBEX(TAU,A,THA,P,  ZB  ,GG)
       RETURN
       END
```

```
$I    FOR  MFST, MFST/FJ
      SUBROUTINE MFST(KFIT,N)
      CALL PAC(KFIT,2,N)
      RETURN
      END
```

```
01    FOR  KFST, KFST/FJ
      SUBROUTINE KFST(KFIT,N)
      CALL PAC(KFIT,1,N)
      RETURN
      END
```

```
      SI  FOR JMK,JMK/FJ
            FUNCTION JMK(K,I)
            CALL UNPACK(K,I,L)
            JMK=L
            RETURN
            END
```

```
BI ASM   PAC
 NBPR .
PAC* .
 L      A0,*2,B11
 L      B13,*1,B11
 AA,016 A1,1
 LSSL   A1,1
 J      $-1,B13
 S,015  A0,*0,B11
 J      4,B11
 S,014  A0,*0,B11
 J      4,B11
 S,013  A0,*0,B11
 J      4,B11
 S,012  A0,*0,B11
 J      4,B11
 S,011  A0,*0,B11
 J      4,B11
 S,010  A0,*0,B11
 J      4,B11
 END
```

```
UI ASM UNPACK
 NBPR .
UNPACK* .
 L      B13,*1,B11
 AA,016 A1,1
 LSSL   A1,1
 J      $-1,B13
 L,015  A0,*0,B11
 J      $+10
 L,014  A0,*0,B11
 J      $+8
 L,013  A0,*0,B11
 J      $+6
 L,012  A0,*0,B11
 J      $+4
 L,011  A0,*0,B11
 J      $+2
 L,010  A0,*0,B11
 S      A0,*2,B11
 J      4,B11
        ENU
```

```
      EQUIVALENCE      (Z(100),HVB),     (Z(101),HCB),     (Z(102),CB),
     1(Z(103),SVS),    (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFL),  (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
     3(Z(111),EZERO),  (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
     3(Z(115),COE),    (Z(116),SCR),     (Z(117),ISR),     (Z(118),SCDR),
     4(Z(119),AHN),    (Z(120),DTH),     (Z(121),IH),      (Z(122),JH),
     5(Z(123),DTC),    (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
     X(Z(127),CDUT),   (Z(128),HCP),     (Z(129),HH),      (Z(130),CO),
     6(Z(131),J1),     (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),     (Z(136),J6),                        (Z(138),SVMAX),
     8(Z(139),FRCDTC)
      EQUIVALENCE      (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
     1(Z(143),SCRE),   (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),     (Z(148),DTVF),    (Z(149),DTUF),    (Z(150),EI1)
C
CC
C
      EQUIVALENCE      (XX(2),X(1)),     (UR,UL,FLEFT),    (UR(100),YAMC),
     1(PR(100),SIGC),  (PR,PL,GAMC),     (UKE,THETA),      (UR,TAB),
     2(UR(16),AMK),    (UR(31),PK),      (UR(46),QK),      (YY(2),Y(1))
C
C              C       O       M       M       O       N
C
C
C     WILL ONLY GENERATE (1) MATERIAL.
C     PACKAGES MUST BE RECTANGLES.
C               Z(14)     FFA       MAX INCREASE IN DT PER CYCLE
C               Z(15)     FFB       MIN POSSIBLE DT
C               Z(25)     FEF       ENERGY FLOW ALLOWABLE
C               Z(65)     SN        ONE ALLOWS NEG I
C               Z(74)     BBOUND    ZERO FOR RADIATION
C               Z(75)     TOZONE    DENSITY LIMIT AT FREE SURFACE
C               Z(77)     SBOUND    WT. FRACTION IN VEL. FOR MASS TRANS.
C     Z(104)    ATOM      ATOMIC NO.
C     Z(110)    ANN       EXP. FOR FN FUNCTION
C     Z(111)    EZERO     INITIAL SOURCE
C     Z(112)    PW        PULSE WIDTH AT HALF MAX
C     Z(113)    CAPS      KS AUSORPTION IN SOLID
C     Z(114)    HNU       LASER PHOTON ENERY
C     Z(115)    COE       CK COEF FOR LOW TEMP
C     A(118)    SCDR      SOURCE DURATION
C     Z,119.    AHN       8.62E10/(ATOM*HNU)**2
C     Z(126)    RFT       REFLECTIVITY
C     Z(127)    CDUT      CONDUCTIVITY
C               Z(138)              SPECIFIC DENSITY CUTOFF
C               Z(139)              PERCENT OF STABILITY FOR DT
      PROB=SPROB
      FFA=2.
      FFB=1.E-10
      FEF=6.
      SN=-1.
      BBOUND=0.
      SBOUND=1.
      SVMAX=1.E+14
      FRCDTC=.5
      CB=CV*(GV-1.)
      AHN = 8.62E10 / (ATOM*HNU)**2
      KMAX=IMAX*JMAX+1                                          SETU1090
      KMAXA=KMAX+1                                              SETU1100
      JMAXA=JMAX+1                                              SETU1110
      IMAXA=IMAX+1                                              SETU1120
      PIDY=3.1415927                                            SETU1230
C               READ IN DY AND DX
      I=0
      J=0
```

```
@I    FOR  SETUP, SETUP/FJ                                              -
      SUBROUTINE SETUP                                                  SETU0010
C
C                D  I  M  E  N  S  I  O  N
C
                          DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),      X(53),       XX(54),      DY(100),     Y(100),     YY(101),
     5TAB(15),     AMK(15),     PK(15),      QK(15),      Z(150),     IZ(150),
     6TAU(52),     PL(200),     PR(200),     UL(200),     UR(200),
     7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12),HEAD(12)
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PIDT6   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,REZ     ,RHO     ,RL
      COMMON          RR,SIG,QUODFL,SWITCH ,TABLM,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          I       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                E  Q  U  I  V  A  L  E  N  C  E
C
     0EQUIVALENCE      (Z,IZ,PROB),     (Z(2),CYCLE),    (Z(3),DT),
     1(Z(4),PRINTS),   (Z(5),PRINTL),   (Z(6),DUMPT7),   (Z(7),CSTOP),
     2(Z(8),PIDY),     (Z(9),TMZ),      (Z(10),SCYCLE),  (Z(11),SPROB),
     3(Z(12),GAMX),    (Z(13),ETH),     (Z(14),FFA),     (Z(15),FFB),
     4(Z(16),TMDZ),    (Z(17),TMXZ),    (Z(18),XMAX),    (Z(19),TXMAX),
     5(Z(20),TYMAX),   (Z(21),AMDM),    (Z(22),AMXM),    (Z(23),DNN),
     6(Z(24),DMIN),    (Z(25),FEF),     (Z(26),DTNA),    (Z(27),CVIS),
     7(Z(28),NPR),     (Z(29),NPRI),    (Z(30),NC),      (Z(31),NPC),
     8(Z(32),NRC),     (Z(33),IMAX),    (Z(34),IMAXA),   (Z(35),JMAX),
     9(Z(36),JMAXA),   (Z(37),KMAX),    (Z(38),KMAXA),   (Z(39),NMAX)
     0EQUIVALENCE      (Z(40),ND),      (Z(41),KDT),     (Z(42),IXMAX),
     1(Z(43),NOD),     (Z(44),NOPR),    (Z(45),NIMAX),   (Z(46),NJMAX),
     2(Z(47),I1),      (Z(48),I2),      (Z(49),I3),      (Z(50),I4),
     3(Z(51),N1),      (Z(52),N2),      (Z(53),N3),      (Z(54),N4),
     4(Z(55),N5),      (Z(56),N6),      (Z(57),N7),      (Z(58),N8),
     5(Z(59),N9),      (Z(60),N10),     (Z(61),N11),     (Z(62),NRM),
     6(Z(63),TRAD),    (Z(64),XNRG),    (Z(65),SN),      (Z(66),DXN),
     7(Z(67),RADER),   (Z(68),RADET),   (Z(69),RADEB),   (Z(70),DTRAD),
     8(Z(71),REZFCT),  (Z(72),RSTOP),   (Z(73),SHELL),   (Z(74),BBOUND),
     9(Z(75),TOZONE),  (Z(76),ECK),     (Z(77),SBOUND),  (Z(78),X1)
     0EQUIVALENCE      (Z(79),X2),      (Z(80),Y1),      (Z(81),Y2),
     1(Z(82),CABLN),   (Z(83),VISC),    (Z(84),T),       (Z(85),GMAX),
     2(Z(86),WSGD),    (Z(87),WSGX),    (Z(88),GMADR),   (Z(89),GMAXR),
     3(Z(90),S1),      (Z(91),S2),      (Z(92),S3),      (Z(93),S4),
     4(Z(94),S5),      (Z(95),S6),      (Z(96),S7),      (Z(97),S8),
     5(Z(98),S9),      (Z(99),S10)
C
```

```
      X(I)=0.
      Y(J)=0.
 2000 READ          ( 5,8102)IWSA,IWSB,N1,N2,N3,N4,( AMX(K),K=1,4)
      L=1
      IF(N4)2003,2001,2003
 2001 IF(N3)2004,2002,2004
 2002 IF(N2)2006,2008,2006
 2003 L=L+1
 2004 L=L+1
 2006 L=L+1
C     TEST TO CALC (X AND DX  IF IWSB=0   OR   Y AND DY  IF IWSB=1)
 2008 IF(IWSB)2010,2010,2030
C     CALC THE  X  AND  DX  VALUES
 2010 DO 2014 N=1,L
      NK=IZ(N+50)
      DO 2012 K=1,NK
      I=I+1
      DX(I)= AMX(N)
      X(I)=X(I-1)+DX(I)
 2012 CONTINUE
 2014 CONTINUE
      GO TO 2050
C     CALC THE  Y  AND  DY  VALUES
 2030 DO 2034 N=1,L
      NK=IZ(N+50)
      DO 2032 K=1,NK
      J=J+1
      DY(J)= AMX(N)
      Y(J)=Y(J-1)+DY(J)
 2032 CONTINUE
 2034 CONTINUE
C     TEST IF ANOTHER CARD SHOULD BE READ (YES IF IWSA=0, NO IF IWSA=1)
 2050 IF(IWSA.EQ.0) GO TO 2000
      WS=X(1)**2
      TAU(1)=WS*P1DY                                                  SETU1240
      DO 2054 I=2,IMAX
      WSA=X(I)**2                                                     SETU1280
      TAU(I)=P1DY*(WSA-WS)                                            SETU1290
      WS=WSA                                                          SETU1300
 2054 CONTINUE
      WRITE (6,8066)IMAX,(DX(I),I=1,IMAX)
      WRITE (6,8067)JMAX,(DY(I),I=1,JMAX)
      WRITE (6,8092)(IMAX,(TAU(I),I=1,IMAX))
C     CLEAR ALL CELL ARRAYS.
      DO 1 K=1,KMAX                                                   SETU1130
      U(K)=0.0                                                        SETU1140
      V(K)=0.0                                                        SETU1150
      P(K)=0.0                                                        SETU1160
      AMX(K)=0.0                                                      SETU1170
      AIX(K)=0.0                                                      SETU1180
      THETA(K)=0.
    1 CONTINUE                                                        SETU1190
      N1=0
      N2=0
      N3=0
      N4=0
      NF=1
      NN=ANN
      DO 10 N1=1,NN
   10 NF=NF*N1
      NP=NN+1
      DO 40 MP=1,NP
      M=MP-1
      MF=1
      DO 20 N1=1,M
```

```
   20 MF=MF*N1
      NMM=NN-M
      NMMF=1
      DO 30 N1=1,NMM
   30 NMMF=NMMF*N1
      ANF=NF
      AMF=MF
      ANMF=NMMF
      AM=M
   40 BNN=(-1.)**M*ANF/(AMF*ANMF*(2.*AM+1.))+BNN
      AAN=ANN
      IF(AAN.EQ.0.) AAN=1.
      TEMP(1)=1./2.**(1./AAN)
      IF(ANN.EQ.0.) TEMP(1)=0.
      TEMP(2)=1.-TEMP(1)
      SCDR=PW/TEMP(2)
      TEMP(3)=SQRT(PIDY*2.*PW*CV/(CDUT*SVS*TEMP(2)))
      IF(CDUT.EQ.0.) TEMP(3)=0.
      TEMP(4)=CDUT*HCB/(2.*(1.-RFT)*CV)
      TEMP(5)=1./((ANN+1.)*BNN*EZERO)
      EXD= 1./(ANN+.5)
      TC = PW/(2.*TEMP(2))*(TEMP(3)*TEMP(4)*TEMP(5))**EXD
      EXD=1./(ANN+1.)
      IF(CDUT.EQ.0.) TC =SCDR/2.*(HCB*2./(EZERO*CAPS))**EXD)
C     CO=SOUND SPEED
      CO=SQRT(GV*(GV-1.)*HCP)
      HH=HVB+HCB-HCP+GV*(GV+1.)*HCP*.5
      T=DY(J5)*(GV-1.)/((GV+1.)*CO)
      DT=T/4.0
      DTNA=DT/Z(139)
      T=T+TC
      TMTC= T-TC
      SCRT=.5*EZERO*(2.*T/SCDR)**(ANN+1.)/TMTC
      IF(T.GT.0.5*SCDR) SCRT= EZERO*(1.-.5*(2.*(1.-T/SCDR))**(ANN+1.))
     1   /TMTC
      SCRTC=     .5*EZERO*(2.*TC/SCDR)**(ANN+1.)/TMTC
      SCR=SCRT-SCRTC
      RSCR=(1.-RFT)*SCRTC*(ANN+1.)*TMTC/TC
      TEMP(1)=(1.-RFT)*SCRTC*TMTC*SVS/HCB*4.0/PIDY
      TEMP(2)=TMTC*SVS*SCR/(HH-HCB)
      IF(CDUT.EQ.0.) TEMP(2)=0.
      TEMP(3)=CDUT*HH*HCB/(CV*(HH-HCB)*(1.-RFT)*SCRTC)*PIDY/4.0
      J=J5
      DO 3050 I=1,ISR
      K=(J-1)*IMAX+I+1
      JB=(I-1)*20+1
      V(K)=- CO*(GV+1.)/GV
      AIX(K)=HH-0.5*V(K)**2
      SOLID(JB+1) =TEMP(1)+(-TEMP(2)+TEMP(3))/(1.+TEMP(3)/(2.*TEMP(1)))
      SOLID(JB+2)=(SCR-HCB*(SOLID(JB+1)-TEMP(1))/(SVS*TMTC))*(1.-HCB/HH)
      SOLID(JB+3) = (1.-RFT)*SCRTC*TMTC + HCB*(SOLID(JB+1)-TEMP(1))/SVS
      SOLID(JB+6)= SOLID(JB+2)/ (HH-HCB)
      AMX(K)=SOLID(JB+6)*(TMTC)*TAU(I)
      RHO(K)=AMX(K)/(TAU(I)*DY(J))
      SCRE = SCRT*TMTC *TAU(I) + SCRE
      RADE=RFT*SCRTC*TMTC*TAU(I) +RADE
       CNDE=SOLID(JB+3)*TAU(I)+CNDE
      W2(I)=SCR
      SOLID(JB+7)=SOLID(JB+6)* TMTC
      VAPE = SOLID(JB+2)*TMTC*TAU(I)+ VAPE+HCB*SOLID(JB+7)*TAU(I)
      SOLID(JB+8)=SCRT*TMTC
      SOLID(JB+4) = SOLID(JB+8)
      SOLID(JB+11)=SOLID(JB+6)*CO/GV
      SOLID(JB+15)=-CO
      SOLID(JB+12)=SOLID(JB+11)+SOLID(JB+6)*ABS(SOLID(JB+15))
```

```
      SOLID(JB+13)=SOLID(JB+12)*(TMTC)
      IF(I.NE.ISR) GO TO 3040
      AMX(K+1) = (GV-1.)/(GV+1.)*AMX(K)/(1.-DX(I)/(2.*X(I)))
     1          * (2./(GV+1.))**(2./(GV-1.))
      AMX(K)=AMX(K)-AMX(K+1)
      AIX(K+1)=HVB+HCB-HCP
      U(K+1) = CO/(GV-1.)
      U(K) =CO/8.
      V(K+1)=-SQRT(2.*(HH-AIX(K+1)) -U(K+1)**2)
      RHO(K)= AMX(K)/(TAU(I)*DY(J))
      RHO(K+1)=AMX(K+1)/(TAU(I+1)*DY(J))
      AIX(K)=AIX(K)-0.5*(U(K)**2)
      ETH = ETH +(AIX(K+1)+ (V(K+1)**2 +U(K+1)**2)/2.)* AMX(K+1)
      SV =1./RHO(K+1)
      CALL ES(SV,AIX(K+1),THETA(K+1),P(K+1),CAP(K+1),GG)
      CALL MFST(KFIT(K+1),1)
 3040 ETH = ETH +(AIX(K)+(V(K)**2+U(K)**2)/2.)*AMX(K)
      SV=1./RHO(K)
      CALL ES(SV,AIX(K),THETA(K),P(K),CAP(K),GG)
      CALL MFST(KFIT(K),1)
 3050 CONTINUE
      DO 2999 I=1,IMAX
      CALL DJLOW(JLOW,JHIGH)
      DO 2999 J=JLOW,JHIGH
      K=(J-1)*IMAX+I+1
      CALL FLAG(KFLAG,JLOW,JHIGH)
      CALL KFST(KFIT(K),KFLAG)
 2999 CONTINUE
      CYCLE=0.0                                                    SETU1550
      DTH=1.E10
      DTC=1.E10
      XMAX=X(IMAX)                                                 SETU1620
      YMAX=Y(JMAX)                                                 SETU1640
      REWIND 10
      WS=555.0                                                     SETU1670
      WRITE(10) WS,CYCLE,PROB
      WRITE(10)(Z(I),I=1,150)
      WRITE(10)(U(I),V(I),AMX(I),AIX(I),P(I),THETA(I),
     1 RHO(I),FIOUT(I),CAP(I),KFIT(I),I=1,KMAXA)
      WRITE(10) X(0),(X(I),TAU(I),I=1,IMAX)
      WRITE(10)(Y(I),I=0,JMAX)
      WS=666.0                                                     SETU1730
      WRITE(10) WS,WS,WS
      REWIND 10
      RETURN                                                       SETU1760
 8102 FORMAT(2I1,4I2,4E10.4)
 8066 FORMAT(1H /11H DX(I) I=1,I2/(5F16.6))
 8067 FORMAT(1H /11H DY(J) J=1,I3/(5F16.6))
 8092 FORMAT(1H /13H AREA(I) I=1,I2/(5F16.6))
      END                                                          SETU1770
```

```
WI    FOR  ESK, ESK/FO
      SUBROUTINE ESK(THA,SV,HNU,CAPK)
      COMMON // Z
C                 E  Q  U  I  V  A  L  E  N  C  E
C
      EQUIVALENCE       (Z(1),PROB),      (Z(2),CYCLL),     (Z(3),DT),
     1(Z(4),PRINTS),    (Z(5),PRINTL),    (Z(6),DUMPTT),    (Z(7),CSTOP),
     2(Z(8),PIDT),      (Z(9),IMZ),       (Z(10),SCYCLL)    (Z(11),SPROB),
     3(Z(12),GAMX),     (Z(13),ETID),     (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),IMDZ),     (Z(17),IMX2),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),    (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),     (Z(25),FCF),      (Z(26),DTHA),     (Z(27),CVIS),
     7(Z(28),NPR),      (Z(29),NPRT),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),      (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),    (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
      EQUIVALENCE       (Z(40),NN),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),      (Z(44),NOPR),     (Z(45),NDMAX),    (Z(46),NJMAX),
     2(Z(47),I1),       (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),       (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),       (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),       (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),     (Z(64),XBRG),     (Z(65),SM),       (Z(66),DXN),
     7(Z(67),RADER),    (Z(68),RADET),    (Z(69),RADER),    (Z(70),DTRAD),
     8(Z(71),REZFCT),   (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),HBOUND),
     9(Z(75),TOZONE),   (Z(76),ECK),      (Z(77),SHOUND),   (Z(78),X1)
      EQUIVALENCE       (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),    (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSBD),     (Z(87),WSBX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),       (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),       (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),       (Z(99),S10)
C
      EQUIVALENCE       (Z(100),RVB),     (Z(101),RCB),     (Z(102),CD),
     1(Z(103),SVS),     (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
     2(Z(107),SUMFE),   (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
     3(Z(111),EZERO),   (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
     3(Z(115),COE),     (Z(116),SCR),     (Z(117),ISR),     (Z(118),SCDR),
     4(Z(119),AHN),     (Z(120),DTH),     (Z(121),IH),      (Z(122),JH),
     5(Z(123),DTC),     (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
     X(Z(127),CDUT),    (Z(128),HCP),     (Z(129),HH),      (Z(130),CO),
     6(Z(131),J1),      (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
     7(Z(135),J5),      (Z(136),J6),                        (Z(138),SVMAX),
     8(Z(139),FRCDTC)
      EQUIVALENCE       (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
     1(Z(143),SCRE),    (Z(144),IV),      (Z(145),JV),      (Z(146),IU),
     2(Z(147),JU),      (Z(148),DTVF),    (Z(149),DTUF),    (Z(150),EI1)
C     REVISED CALCULATION OF CAPK IN ESK  7/19/66
      ZBAR=CAPK
      SCLIM=0.4*ZBAR/ATOM
      IF(THA.GT.2.0) GO TO 10
      CPL1=COE*(THA/SV)**2*THA**2
      CAPL2=AMIN1(CPL1+SCLIM,CAPS)
      IF(THA.GT.1.) GO TO 20
      CAPK=CAPL2
      GO TO 1000
   10 CPL3=8.62E10*ZBAR**2*AMAX1(1.,ZBAR)*(FREXP(HNU/
     1THA)-1.)/(SV*SQRT(THA)*ATOM**2*HNU**3)
      CAPK=AMAX1(CPL3,SCLIM)
      GO TO 1000
   20 CPL4=8.81E8*THA*FREXP(-EI1/THA)*(1.0-
     1FREXP(-HNU/THA))/(ATOM*HNU**3)
      CAPK=AMAX1(CAPL2,CPL4)
 1000 RETURN
      END
```

```
WI    FOR SPRINT, SPRINT/FJ
      SUBROUTINE SPRINT
C
C                D I M E N S I O N
C
                      DIMENSION
     1U(1200),     V(1200),     AMX(1200),   AIX(1200),   P(1200),
     2THETA(1200), RHO(1200),   FIOUT(1200), CAP(1200),   KFIT(1200),
     3PUL(255),IW1(50),W2(50),W3(50),TABLM(50),
     4DX(52),    X(53),      XX(54),     DY(100),    Y(100),     YY(101),
     5TAB(15),   AMK(15),    PK(15),     QK(15),     Z(150),     IZ(150),
     6TAU(52),   PL(200),    PR(200),    UL(200),    UR(200),
     7HLEFT(100),YAMC(100),SIGC(100),GAMC(100),
     8G(50),SOLID(400),TEMP(12), HEAD(12)
      COMMON          Z       ,XX      ,UR      ,PR      ,THETA   ,YY
      COMMON          AID     ,AIX     ,AM      ,AMD     ,AMX     ,AREA
      COMMON          BIG     ,BOUNCE  ,DDXN    ,DDVK    ,DVK     ,DX
      COMMON          DY      ,E       ,FD      ,FS      ,FX      ,OUT
      COMMON          P       ,PABOVE  ,PBLO    ,PTOTS   ,PPABOV  ,PRR
      COMMON          PUL     ,QDT     ,RC      ,R       ,RHO     ,RL
      COMMON          RR,SIG,GOOFL,SWITCH ,TABL  ,TAU
      COMMON          TAUDTS  ,TAUDTX  ,U       ,UK      ,URR     ,UT
      COMMON          UU      ,UUU     ,UTEF    ,UVMAX   ,V       ,VABOVE
      COMMON          VBLO    ,VEL     ,VK      ,VT      ,VTEF    ,VV
      COMMON          VVABOV  ,VVBLO   ,W2      ,W3      ,WPS     ,WS
      COMMON          WSA     ,WSB     ,WSC     ,XL      ,XLF     ,XN
      COMMON          XR      ,YL      ,YLW     ,YN      ,YU      ,ZMAX
      COMMON          1       ,II      ,IN      ,IR      ,IWS     ,IWSA
      COMMON          IWSB    ,IWSC    ,IW1     ,J       ,JN      ,JP
      COMMON          JR      ,K       ,KN      ,KP      ,KR      ,KRM
      COMMON          L       ,M       ,MA      ,MB      ,MC      ,MD
      COMMON          ME      ,MZ      ,N       ,NK      ,NKMAX   ,NK1
      COMMON          NO      ,NR      ,G       ,SOLID   ,TEMP
      COMMON          FIOUT   ,CAP     ,KFIT    ,ISEND   ,IGOTO   ,HEAD
C
C
C                E Q U I V A L E N C E
C
     0EQUIVALENCE       (Z,IZ,PROB),      (Z(2),CYCLE),     (Z(3),DT),
     1(Z(4),PRINTS),    (Z(5),PRINTL),    (Z(6),DUMPT7),    (Z(7),CSTOP),
     2(Z(8),PIDY),      (Z(9),TMZ),       (Z(10),SCYCLE),   (Z(11),SPROB),
     3(Z(12),GAMX),     (Z(13),ETH),      (Z(14),FFA),      (Z(15),FFB),
     4(Z(16),TMDZ),     (Z(17),TMXZ),     (Z(18),XMAX),     (Z(19),TXMAX),
     5(Z(20),TYMAX),    (Z(21),AMDM),     (Z(22),AMXM),     (Z(23),DNN),
     6(Z(24),DMIN),     (Z(25),FEF),      (Z(26),DTNA),     (Z(27),CVIS),
     7(Z(28),NPR),      (Z(29),NPR1),     (Z(30),NC),       (Z(31),NPC),
     8(Z(32),NRC),      (Z(33),IMAX),     (Z(34),IMAXA),    (Z(35),JMAX),
     9(Z(36),JMAXA),    (Z(37),KMAX),     (Z(38),KMAXA),    (Z(39),NMAX)
     0EQUIVALENCE       (Z(40),ND),       (Z(41),KDT),      (Z(42),IXMAX),
     1(Z(43),NOD),      (Z(44),NOPR),     (Z(45),NIMAX),    (Z(46),NJMAX),
     2(Z(47),I1),       (Z(48),I2),       (Z(49),I3),       (Z(50),I4),
     3(Z(51),N1),       (Z(52),N2),       (Z(53),N3),       (Z(54),N4),
     4(Z(55),N5),       (Z(56),N6),       (Z(57),N7),       (Z(58),N8),
     5(Z(59),N9),       (Z(60),N10),      (Z(61),N11),      (Z(62),NRM),
     6(Z(63),TRAD),     (Z(64),XNRG),     (Z(65),SN),       (Z(66),DXN),
     7(Z(67),RADER),    (Z(68),RADET),    (Z(69),RADEB),    (Z(70),DTRAD),
     8(Z(71),RLZFCT),   (Z(72),RSTOP),    (Z(73),SHELL),    (Z(74),DBOUND),
     9(Z(75),TOZONE),   (Z(76),ECK),      (Z(77),SBOUND),   (Z(78),X1)
     0EQUIVALENCE       (Z(79),X2),       (Z(80),Y1),       (Z(81),Y2),
     1(Z(82),CABLN),    (Z(83),VISC),     (Z(84),T),        (Z(85),GMAX),
     2(Z(86),WSGD),     (Z(87),WSGX),     (Z(88),GMADR),    (Z(89),GMAXR),
     3(Z(90),S1),       (Z(91),S2),       (Z(92),S3),       (Z(93),S4),
     4(Z(94),S5),       (Z(95),S6),       (Z(96),S7),       (Z(97),S8),
     5(Z(98),S9),       (Z(99),S10)
C
```

```
      EQUIVALENCE     (Z(100),HVB),    (Z(101),HCB),    (Z(102),CB),
     1(Z(103),SVS),   (Z(104),ATOM),   (Z(105),CV),     (Z(106),GV),
     2(Z(107),SUMFE), (Z(108),BETA),   (Z(109),ALCO),   (Z(110),ANN),
     3(Z(111),EZERO), (Z(112),PW),     (Z(113),CAPS),   (Z(114),HNU),
     3(Z(115),COE),   (Z(116),SCR),    (Z(117),ISR),    (Z(118),SCDR),
     4(Z(119),AHN),   (Z(120),DTH),    (Z(121),IH),     (Z(122),JH),
     5(Z(123),DTC),   (Z(124),IC),     (Z(125),JC),     (Z(126),RFT),
     X(Z(127),CDUT),  (Z(128),HCP),    (Z(129),HH),     (Z(130),CO),
     6(Z(131),J1),    (Z(132),J2),     (Z(133),J3),     (Z(134),J4),
     7(Z(135),J5),    (Z(136),J6),                      (Z(138),SVMAX),
     8(Z(139),FRCDTC)
      EQUIVALENCE     (Z(140),VAPE),   (Z(141),RADE),   (Z(142),CNDE),
     1(Z(143),SCRE),  (Z(144),IV),     (Z(145),JV),     (Z(146),IU),
     2(Z(147),JU),    (Z(148),DTVF),   (Z(149),DTUF),   (Z(150),EI1)
C
      EQUIVALENCE     (XX(2),X(1)),    (UR,UL,FLLFT),   (UR(100),YA4C),
     1(PR(100),SIGC), (PR,PL,GAMC),    (DKE,THETA),     (UR,TAB),
     2(UR(16),AMK),   (UR(51),PK),     (UR(46),QK),     (YY(2),Y(1))
      COMMON/HEADER/ TITLE(48), TITLE1(48), TITLE2(48), TITLE3(6)
      DATA  TITLE/288HPROB  CYCLE DT    PRINTSPRINTLDUMPT7CSTOP PIDY  TM
     1Z    SCYCLESPROB GAMX  ETH   FFA   FFB   TMDZ  TMXZ  XMAX  TXMAX TY
     2MAX AMDM  AMXM  DNN   DMIN  FEF   DTNA  CVIS  NPR   NPRI  NC    NP
     3C    NRC   IMAX  1MAXA JMAX  JMAXA KMAX  KMAXA NMAX  ND    KDT   IX
     4MAX NOD   NOPR  N1MAX NJMAX I1    I2    /
      DATA TITLE1/288HI3    I4    N1    N2    N3    N4    N5    N6    N7
     1     N8    N9    N10   N11   NRM   TRAD  XNRG  SN    DXN   RADER RA
     2DET RADEB DTRAD REZFCTRSTOP SHELL BBOUNDTOZONEECK   SBOUNDX1    X2
     3     Y1    Y2    CABLN VISC  T     GMAX  WSGD  WSGX  GMADR GMAXR S1
     4     S2    S3    S4    S5    S6    S7    /
      DATA TITLE2/288HS8    S9    S10   HVB   HCB   CB    SVS   ATOM  CV
     1     GV    SUMFE BETA  ALCO  ANN   EZERO PW    CAPS  HNU   COE   SC
     2R   ISR   SCDR  AHN   DTH   IH    JH    DTC   IC    JC    RFT   CD
     3UT  HCP   HH    CO    J1    J2    J3    J4    J5    J6          SV
     4MAX FRCDTCVAPE  RADE  CNDE  SCRE  IV    /
      DATA TITLE3/36HJV     IU    JU    DTVF  DTUF  EI1   /
      IGO=1
      KOUNT=1
      IFROM=1
      ITO=8
      WRITE(6,10) (HEAD(I),I=1,12),CYCLE
   10 FORMAT(37H1 HECTIC PANIC DUMP OF PROBLEM . . . 12A6,5HCYCLEF6.0)
      WRITE(6,3) S1
    3 FORMAT(7H  S1 = F10.4)
   15 WRITE(6,20) (TITLE(I),I=IFROM,ITO)
   20 FORMAT(1H0 / 5X,8A15)
      GO TO (22,22,22,24,26,26),IGO
   22 WRITE(6,23)KOUNT,(Z(I),I=IFROM,ITO)
      GO TO 30
   23 FORMAT(1X,I5,1P8E15.7)
   24 WRITE(6,25)KOUNT,(Z(I),I=IFROM,ITO)
   25 FORMAT(1X,I5,1P3E15.7,5(5X,I10))
      GO TO 30
   26 WRITE(6,27)KOUNT,(Z(I),I=IFROM,ITO)
   27 FORMAT(1X,I5,8(5X,I10))
   30 IGO=IGO+1
      KOUNT=KOUNT+8
      IFROM=IFROM+8
      ITO=ITO+8
      IF(IGO.LT.7) GO TO 15
      IGO=1
   31 WRITE(6,20) (TITLE(I),I=IFROM,ITO)
      GO TO (32,34,36,36,36,36),IGO
   32 WRITE(6,27)KOUNT,(Z(I),I=IFROM,ITO)
      GO TO 40
   34 WRITE(6,35)KOUNT,(Z(I),I=IFROM,ITO)
```

```
   35 FORMAT(1X,I5,6(5X,I10),1P2E15.7)
      GO TO 40
   36 WRITE(6,23)KOUNT,(Z(I),I=IFROM,ITO)
   40 IGO=IGO+1
      IFROM=IFROM+8
      ITO=ITO+8
      KOUNT=KOUNT+8
      IF(IGO.LT.7) GO TO 51
      IGO=1
   41 WRITE(6,20) (TITLE(I),I=IFROM,ITO)
      GO TO (42,42,44,46,48,42),IGO
   42 WRITE(6,23)KOUNT,(Z(I),I=IFROM,ITO)
      GO TO 50
   44 WRITE(6,45)KOUNT,(Z(I),I=IFROM,ITO)
   45 FORMAT(1X,I5,1P4E15.7,5X,I10,3E15.7)
      GO TO 50
   46 WRITE(6,47)KOUNT,(Z(I),I=IFROM,ITO)
   47 FORMAT(1X,I5,2(5X,I10),1PE15.7,2(5X,I10),3E15.7)
      GO TO 50
   48 WRITE(6,49)KOUNT,(Z(I),I=IFROM,ITO)
   49 FORMAT(1X,I5,1P2E15.7,6(5X,I10))
   50 IGO=IGO+1
      IFROM=IFROM+8
      ITO=ITO+8
      KOUNT=KOUNT+8
      IF(IGO.LT.7) GO TO 41
      WRITE(6,20) (TITLE(I),I=145,150)
      WRITE(6,23)KOUNT,(Z(I),I=145,150)
      WRITE(6,111)
      WRITE(6,112)
      WRITE(6,113)
      WRITE(6,114)
      WRITE(6,115)
      WRITE(6,116)
      IF(S1-4.0108)53,54,52
   52 IF(S1-4.0126)53,54,53
   53 IF(ABS(ECK).GT.DMIN) WRITE(6,117) ECK,DMIN
  111 FORMAT(79H1S1                    ERROR NUMBER TO FLAG THE SUBROUTINE WH
     1ICH CALLED MACHINE EXIT)
  112 FORMAT(53H0                      4.0108 NORMAL EXIT AFTER MAX. CYCLE//)
  113 FORMAT(89H                       1. MAIN          5. CDT          9. PH2
     1          13. ES          17. PAC   )
  114 FORMAT(89H                       2. CARDS         6. SCRC         10. FLA
     1G          14. JMR         18. SETUP)
  115 FORMAT(89H                       3. INPUT         7. BOIL         11. DJL
     10W         15. MFST        19. ESK   )
  116 FORMAT(89H                       4. EDIT          8. PH1          12. LIB
     1EX         16. KFST        20.       )
  117 FORMAT(28H0  ENERGY CHECK ERROR. ECK =1PE15.7,7H DMIN =E15.7)
   54 REWIND 10
      IF(N7.EQ.10) GO TO 1000
      REWIND N7
 1000 CALL EXIT
      END
```

REFERENCES

1. Tillotson, J. H., "Metallic Equations of State for Hypervelocity Impact," General Atomic Report GA-3216, July, 1962, p. 12.
2. Carslaw, H. S., and J. C. Jaeger, Conduction of Heat in Solids, Oxford Press, 2nd Ed., 1959, p. 76.

SECTION III
EQUATIONS OF STATE FOR IONIZED VAPOR

3.1. INTRODUCTION

Theoretical studies of hydrodynamics and radiation transport require information about the thermodynamic state variables of the system. In many applications, local thermodynamic equilibrium (LTE) may be assumed. Under this assumption, the law of mass action can be used to solve for the equilibrium concentrations of every species present in the system.

The methods described in this section, and the EIONX computer routines based upon them, apply to equilibria involving neutral atoms, ions, and electrons. At low temperatures (generally less than 2 ev), molecular constituents may also be present. Their equilibria, however, are calculated by other methods. The EIONX codes provide for linkage of molecular equilibrium routines in such a way that the contribution of the latter to the thermodynamic properties of the system can be taken into account.

The law of mass action was applied by Saha in 1920 to the equilibrium

$$Cs \rightleftharpoons Cs^{+} + e^{-} .$$

With concentrations, in cm^{-3}, of neutrals, ions, and electrons denoted, respectively, by $[Cs]$, $[Cs^{+}]$ and $[e^{-}]$, the law states that for equilibrium at $T^{o}K$,

$$\frac{[e]\ [Cs^{+}]}{[Cs]} = e^{-\Delta G(T)/kT}$$

where $\Delta G(T)$ is the free energy change in the reaction. Similar relationships hold for equilibrium concentrations of more highly ionized stages and excited ionic states. If the perfect gas law is assumed, the following general relationship can be shown to hold for the relative concentrations or mole fractions, X_j, of ions of some atomic species in stage j (ionic charge je):

$$\frac{X_j}{X_{j-1}} = \Gamma \frac{u_j}{u_{j-1}} e^{-V_j/kT}$$

where V_j is the jth ionization potential of the atom, u_j is the partition function for stage j, and Γ is a parameter which is inversely proportional to the electron density, and therefore depends on the concentrations of all ionization stages of every atomic species present.

The calculation of the state of the vapor at a given temperature and mass density therefore involves solution of a comparatively extensive system of coupled nonlinear equations for the concentrations of each constituent. The EIONX routines perform this task, with the aid of certain simplifying assumptions, and then proceed to the evaluation of the thermodynamic state variables of the system. These simplifying assumptions are most valid in those regions of phase space (essentially characterized by $\Gamma \gg 1$) in which particle interactions are sufficiently infrequent that the distribution of ionic states is sharply peaked. In other regions, not only these assumptions but also those more basic ones mentioned in the preceding paragraph are likely to be invalid.

3.2. FORMULATION OF THE LINEAR EIONX ROUTINES

3.2.1. Definitions

τ	Specific volume, $cm^3 g^{-1}$,
θ	Temperature, ev; $\theta = kT$,
P	Pressure, dynes cm^{-2},
E	Specific internal energy, ergs g^{-1},

α_i Number fraction of element i in the material;

$$\sum_i \alpha_i = 1,$$

Z^i Atomic number of element i,

V_j^i j^{th} ionization potential of element i,

X_j^i Number fraction of element i in the j^{th} ionization stage; $\sum_j X_j^i = 1$

$\bar{Z}^i$ Mean ionic charge of element i; $\bar{Z}^i = \sum_{j=1}^{Z^i} j X_j^i$,

$\bar{Z}$ Mean ionic charge of material; $\bar{Z} = \sum_i \alpha_i \bar{Z}^i$,

A_i Atomic mass number of element i,

$\bar{A}$ Mean atomic mass number; $\bar{A} = \sum_i \alpha_i A_i$,

φ Gas constant in ergs $g^{-1} ev^{-1}$; $\varphi = eR/k\bar{A} = eN_o/\bar{A}$

$$\cong 9.65 \times 10^{11}/\bar{A},$$

c Constant in Saha equation; $c = 2h^{-3}(2\pi m_e)^{3/2} m_p eR/k$

$$\cong e^{22.99} \text{ergs ev}^{-5/2} \text{cm}^{-3},$$

Γ Electronic "nondegeneracy" parameter;

$$\Gamma = c\tau\theta^{3/2}/\varphi\bar{Z},$$

I^o $I^o = \theta \ln (c\tau\theta^{3/2}/\varphi)$,

β_j^i $\beta_j^i = \exp[(I^o - V_j^i)/\theta]$,

I $I = \theta \ln \Gamma = I^o - \theta \ln \bar{Z}$,

$\bar{N}$ Mean number of atoms per molecule.

3.2.2. The Saha Equation for Ionic Equilibria

$$\frac{X^i_j}{X^i_{j-1}} = \Gamma e^{-V^i_j/\theta} = e^{(I-V^i_j)/\theta} = \frac{\beta^i_j}{\bar{Z}} \qquad 1 \le j \le Z^i$$

The ratio of partition functions u_j/u_{j-1} has been omitted from this equation. It is usually of order unity, in contrast to Γ and the exponential factor. The effect of omitting this ratio is thus equivalent to a small shift in temperature. The pressure lowering of the ionization potential is also neglected.

It should be noted that the distribution of populations X^i_j is in general strongly peaked near those stages j for which $V^i_j \simeq I$. For $V^i_j = I$, in particular, X^i_j and X^i_{j-1} are equal, while the adjacent terms X^i_{j+1} and X^i_{j-2} are smaller by factors such as $\exp(-\Delta V/\theta)$, where ΔV, the separation of the ionization potentials, is usually large compared with θ. The mean ionic charge $\bar{Z}^i$, for $I = V^i_j$, is thus approximately

$$\bar{Z}^i \simeq (j-1)\, X^i_{j-1} + j X^i_j \simeq j - 1/2$$

This fact is used as the basis for an approximate interpolation procedure which avoids the need for solving the entire coupled set of Saha equations yet preserves some of the basic characteristics of any such solution, namely, that $\bar{Z}^i$ is a continuous monotonic increasing function of I which assumes half-odd-integer values when I is close to an ionization potential.

3.2.3. The ETONX Model for Mean Ionic Charge

$$\bar{Z}^i = j - \frac{3}{2} + \frac{I - V^i_{j-1}}{V^i_j - V^i_{j-1}}, \qquad V^i_{j-1} < I \leq V^i_j, \; j = 2, \ldots Z^i$$

$$\bar{Z}^i = \left[1 + \exp\left(\frac{V^i_1 - I}{\theta}\right) \right]^{-1} = X^i_1 = \frac{\beta^i_1}{\bar{Z} + \beta^i_1}, \qquad I < V^i_1$$

$$X^i_Z = \left[1 + \exp\left(- \frac{I - V^i_Z}{\theta} \right) \right]^{-1} = \frac{\beta^i_Z}{\bar{Z} + \beta^i_Z}, \qquad I > V^i_Z$$

$$\bar{Z}^i = Z^i - 1 + X^i_Z, \qquad I > V^i_Z$$

That is, for I between two ionization potentials, $\bar{Z}^i(I)$ is the linear interpolant between the half-integer values defined above; and for I less than the first ionization potential or greater than the last, it is assumed that only two ionization stages are populated (the neutral or stripped stage, respectively, and the adjacent stage), in which case a single Saha equation determines the state.

These assumptions, together with the defining relations

$$\bar{Z} = \sum_i \alpha_i \bar{Z}^i$$

$$I = I^o - \theta \ln \bar{Z}$$

form the basis for an iterative solution for I, $\bar{Z}$, and the $\bar{Z}^i$, given θ and τ or I^o.

3.2.4. Computation of P and E

The thermodynamic variables to be computed are the pressure P, the internal energy E, and their derivatives with respect to the independent variables τ and θ. All of these quantities depend upon $\bar{Z}$, as well. Since

$\bar{Z}$ is not an independent variable but a function of τ and θ determined by the model discussed above, it is necessary to impose a thermodynamic consistency condition of some sort on the definitions of P and E. A suitable choice is the thermodynamic relation

$$\left(\frac{\partial E}{\partial \tau}\right)_\theta = \theta \left(\frac{\partial P}{\partial \theta}\right)_\tau - P$$

For the pressure, the perfect gas law is assumed:

$$P = (\bar{N}^{-1} + \bar{Z})\, \varphi\theta/\tau$$

and for the internal energy a sum of random kinetic, ionization, and dissociation terms:

$$E = \frac{3}{2}(\bar{N}^{-1} + \bar{Z})\, \varphi\theta + \varphi \sum_i \alpha_i \mathcal{E}_i + E_{dis}$$

where E_{dis} is the molecular dissociation contribution, and $\mathcal{E}_i$, the mean ionization energy per atom of element i, is

$$\mathcal{E}_i = \sum_{k=1}^{j-1} V_k^i + V_{j-1}^i (\bar{Z}^i - j + 1) + (V_j^i - V_{j-1}^i)(\bar{Z}^i - j + \tfrac{3}{2})^2/2 \qquad V_{j-1}^i < I \le V_j^i$$

$$\mathcal{E}_i = \bar{Z}^i V_1^i \qquad I < V_1^i$$

$$\mathcal{E}_i = \sum_{k=1}^{Z^i - 1} V_k^i + (\bar{Z}^i - Z^i + 1) V_Z^i \qquad I > V_Z^i$$

These definitions for $\mathcal{E}_i$ are the simplest which conform to the thermodynamic consistency condition and also to the assumptions made above for the X_j^i.

The derivatives of P and E are

$$\left(\frac{\partial P}{\partial \theta}\right)_\tau = P/\theta + \frac{\varphi\theta}{\tau}\left[\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_\tau - \bar{N}^{-2}\left(\frac{\partial \bar{N}}{\partial \theta}\right)_\tau\right]$$

$$\left(\frac{\partial P}{\partial \tau}\right)_\theta = -\frac{P}{\tau} + \frac{\varphi\theta}{\tau}\left[\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_\theta - \bar{N}^{-2}\left(\frac{\partial \bar{N}}{\partial \tau}\right)_\theta\right]$$

$$C_V = \left(\frac{\partial E}{\partial \theta}\right)_\tau = \frac{3}{2}\varphi(\bar{N}^{-1} + \bar{Z}) + \frac{3}{2}\varphi\theta\left[\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_\tau - \bar{N}^{-2}\left(\frac{\partial \bar{N}}{\partial \theta}\right)_\tau\right]$$

$$+ \varphi\sum_i \alpha_i\left(\frac{\partial \mathcal{E}_i}{\partial \theta}\right)_\tau + \left(\frac{\partial E_{dis}}{\partial \theta}\right)_\tau$$

$$\left(\frac{\partial E}{\partial \tau}\right)_\theta = \frac{3}{2}\varphi\theta\left[\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_\theta - \bar{N}^{-2}\left(\frac{\partial \bar{N}}{\partial \tau}\right)_\theta\right] + \varphi\sum_i \alpha_i\left(\frac{\partial \mathcal{E}_i}{\partial \tau}\right)_\theta + \left(\frac{\partial E_{dis}}{\partial \tau}\right)_\theta$$

where $\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_\tau = D^{-1}\sum_i \alpha_i\left(\frac{J_i}{\theta} + \frac{3}{2}\right)\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta$

$$\left(\frac{\partial \bar{Z}}{\partial \tau}\right)_\theta = D^{-1}\frac{\theta}{\tau}\sum_i \alpha_i\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta$$

$$\left(\frac{\partial \mathcal{E}_i}{\partial \tau}\right)_\theta = J_i\left(\frac{\partial \bar{Z}^i}{\partial \tau}\right)_\theta = J_i\left[\frac{\theta}{\tau} - \frac{\theta}{\bar{Z}}\left(\frac{\partial \bar{Z}}{\partial \mathcal{E}}\right)_\theta\right]\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta$$

$$\left(\frac{\partial \mathcal{E}_i}{\partial \theta}\right)_\tau = J_i\left(\frac{\partial \bar{Z}^i}{\partial \theta}\right)_\tau = J_i\left[\frac{J_i}{\theta} + \frac{3}{2} - \frac{\theta}{\bar{Z}}\left(\frac{\partial \bar{Z}}{\partial \theta}\right)_\tau\right]\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta$$

$$J_i = \text{Min}\left[V_Z^i,\ \text{Max}\,(V_1^i,\ I)\right]$$

$$D = 1 + \frac{\theta}{\bar{Z}}\sum_i \alpha_i\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta$$

$$\left(\frac{\partial \bar{Z}^i}{\partial I}\right)_\theta = \frac{1}{V_j^i - V_j^{i-1}}, \qquad V_{j-1}^i < I \le V_j^i, \; j = 2, \ldots Z^i$$

$$= \frac{\beta_1^i \bar{Z}}{\theta(\bar{Z} + \beta_1^i)^2} = \frac{X_1^i (1 - X_1^i)}{\theta} \qquad I < V_1^i$$

$$= \frac{\beta_Z^i \bar{Z}}{\theta(\bar{Z} + \beta_Z^i)^2} = \frac{X_Z^i (1 - X_Z^i)}{\theta} \qquad I > V_Z^i$$

E_{dis}, $\bar{N}$, and their derivatives are obtained from molecular equilibrium routines external to EIONX. If no such routines are used, $\bar{N}$ is taken to be 1 and its derivatives are taken to be zero; similarly, $E_{dis} = 0$.

The velocity of sound, c_o, is determined from these derivatives by using the thermodynamic relation

$$c_o^2 = \tau^2 \left[\frac{\theta}{C_V}\left(\frac{\partial P}{\partial \theta}\right)_\tau^2 - \left(\frac{\partial P}{\partial \tau}\right)_\theta\right]$$

3.3. PROCEDURES FOR ITERATIVE SOLUTION

When only one element is present in the material, a number of simplifications are possible in the formulation and in the program coding; furthermore a more efficient iterative procedure is available. Two versions of the linear EIONX routines were therefore prepared. The more general multi-element procedure is described first.

3.3.1. Multi-element Iterative Procedure

1. Initialize (i.e., iteration index n = 1): $\bar{Z}^{(n)} = 1$.
2. $I^o - \theta \ln \bar{Z}_{(n)} \rightarrow I_{(n)}$.

3. Compute $\bar{Z}^i$.

4. $\sum_i \alpha_i \bar{Z}^i \rightarrow \bar{Z}_{(n+1)}$.

5. Apply Aitken extrapolation every third pass.

6. If

$$\left| \frac{\bar{Z}_{(n+1)} - \bar{Z}_{(n)}}{\bar{Z}_{(n+1)}} \right| > \epsilon$$

then $n+1 \rightarrow n$ and repeat from step 2.

7. Otherwise, $I^o - \theta \ln \bar{Z}_{(n+1)} \rightarrow I$.

8. Compute $\bar{Z}$, its derivatives, and all of the thermodynamic variables defined in Section 3.2.

The procedure converges unless, for some i,

$$\frac{\theta / \bar{Z}}{V^i_j - V^i_{j-1}} > 1 \text{ and } 1/2 < \bar{Z} < \bar{Z}^i - 1/2$$

Since, usually, $V^i_j - V^i_{j-1} > 2\theta$, failures are exceptional. They have occasionally been noted for materials at moderately low temperature and very high density, essentially also the conditions for electron degeneracy and consequently for inapplicability of the entire formulation. If convergence does not occur in 20 iterations, a flag is set and the last iterate is used.

3.3.2. Single-element Iterative Procedure

For $V_1 < I \leq V_Z$,

$$\bar{Z} = j - 1.5 + \frac{I^o - \theta \ln \bar{Z} - V_{j-1}}{V_j - V_{j-1}} = a - b \ln \bar{Z}$$

where

$$a = j - 1.5 + \frac{I^{o} - V_{j-1}}{V_j - V_{j-1}}, \qquad b = \frac{\theta}{V_j - V_{j-1}}$$

If $b/\bar{Z} < 1$, the iteration procedure

$$\bar{Z}_{(n+1)} = a - b \ln \bar{Z}_{(n)}$$

converges, since then

$$\bar{Z}_{(n+1)} - \bar{Z}_{(n)} = -b \ln \left[1 + \frac{\bar{Z}_{(n)} - \bar{Z}_{(n-1)}}{\bar{Z}_{(n-1)}} \right]$$

$$\cong -b \frac{\bar{Z}_{(n)} - \bar{Z}_{(n-1)}}{\bar{Z}_{(n-1)}}$$

and the convergence ratio is

$$\left| \frac{Z_{(n+1)} - Z_{(n)}}{Z_{(n)} - Z_{(n-1)}} \right| \cong \frac{b}{\bar{Z}} < 1$$

By a similar argument it can be shown that if $b/\bar{Z} > 1$, the iteration procedure

$$\ln \bar{Z}_{(n+1)} = \frac{a - \bar{Z}_{(n)}}{b}$$

is convergent.

There is, however, a far more efficient procedure for the single-element case. For $V_{j-1} < I \leq V_j$, let $\alpha = j - 1/2$ and $x = (I - V_{j-1})/(V_j - V_{j-1})$ so that $\bar{Z} = \alpha + x$ with $0 < x \leq 1$.

The equation

$$\bar{Z} = a - b \ln \bar{Z}$$

may then be written as

$$\alpha + x = a - b \ln (\alpha + x)$$

so that

$$x = -\alpha + a - b \left[\ln \alpha + 2 \sum_{k=0}^{\infty} \frac{1}{2k+1} \left(\frac{x}{2\alpha + x} \right)^{2k+1} \right]$$

or

$$x = \left(1 + \frac{2b}{2\alpha + x}\right)^{-1} \left[-\alpha + a - b \ln \alpha - 2b \sum_{k=1}^{\infty} \frac{1}{2k+1} \left(\frac{x}{2\alpha + x} \right)^{2k+1} \right]$$

This expansion of the logarithm converges provided that $\alpha > 0$ and $-\alpha < x < +\infty$; both conditions are satisfied in this application. The iterative solution for x is then straightforward:

$$x_{(1)} = -\alpha + a - b \ln \alpha - 2b \frac{x}{2\alpha + x}$$

$$x_{(n+1)} = \left(1 + \frac{2b}{2\alpha + x_{(n)}}\right)^{-1} \left[-\alpha + a - b \ln \alpha - 2b \sum_{k=1}^{3} \frac{1}{2k+1} \left(\frac{x_{(n)}}{2\alpha + x_{(n)}} \right)^{2k+1} \right]$$

This procedure is more than twice as efficient as the general multi-element procedure for a single element, primarily owing to the elimination of most of the logarithm calculations and the bookkeeping required for additional elements.

3.4. PROGRAM FLOW

The EIONX routines are called by

CALL EIONX (X1, X2, M1, X3)

where X1 is the temperature θ in ev; X2 is the specific volume τ in cm^3/g; M1 is a material identification integer discussed below; X3 on entry specifies any special options as discussed below; and X3 on exit contains an error parameter if a noncatastrophic error has occurred, or zero if no error has occurred. Catastrophic errors cause an immediate return with

a nonzero value for the error flag EION(14). The calling program should check both X3 and EION(14) on return, and take appropriate action if either flag was set.

On entry to EIONX, a nonzero value for EION(14) enables a call to one of three molecular equation-of-state routines, provided that the material identifier M1 is set to one of the following:

102	(air)
101	(polyethylene)
306 or 6	(carbon)

The subsequent procedure for air is as follows: M1 is changed from 102 to 208 and a return is made to the calling program, which then calls a specialized air routine. For carbon and polyethylene, the molecular subroutine CMOL (for carbon) or ESILMS (for polyethylene) is called directly for calculation of E_{dis}, $\bar{N}$, and their derivatives. On return to EIONX, $\bar{Z}$ and the other ionic variables are calculated in the same way as in the monatomic case (an approach which is more valid for carbon than for polyethylene, but is considered satisfactory for both materials). The final results contain contributions of both molecular and ionic processes.

3.5. COMMUNICATIONS BLOCKS

Except for the four subroutine parameters, communication with EIONX is handled through arrays in named COMMON blocks. The contents of these are listed below. At the top of each list are the block name, array name, and array dimension; and for each element of the array, the index, equivalent names, and descriptive information, including variable type if different from the implicit type of the name, are given.

/LMS/EION(20): The main output communications region

EION (1) THETA, θ, temperature, ev

(2) TAU, τ, specific volume, cm^3/g

(3) ZBAR, $\bar{Z}$, mean ionic change, or free electrons per atom

(4) ZBARI, $\bar{Z}^i$, mean ionic charge of a constituent element

(5) PHI, φ, gas constant, erg/g/ev

(6) ESUM

(7) PRESHR, P, pressure, dyne/cm^2

(8) ENERGY, E, specific internal energy, erg/g

(9) DEDTHT, $(\partial E/\partial \theta)_\tau = C_V$, specific heat at constant volume

(10) DEDTAU, $(\partial E/\partial \tau)$

(11) SNDSPD, $\tau(-\partial P/\partial \tau)_S^{\frac{1}{2}} = c_o$, sound speed

(12) DPDTAU, $(\partial P/\partial \tau)_\theta$

(13) DPDTHT, $(\partial P/\partial \theta)_\tau$

(14) If nonzero input, molecular EOS is called; if nonzero output, fatal error.

(15)

(16) ZMEAN, $\Sigma_i \alpha_i Z$, mean atomic number of elements in the material

(17) NBAR, $\bar{N}$, mean number of atoms per molecule; REAL type

(18) ZSUM1

(19) ZSUM2

(20) ZSUM3

/LMSB/U(1): A variable-length input block, supplied by the MARI routine. Any number of elements, greater or equal to those actually needed, may be represented, and in any order; preferably those used most should be first. In the MARI routine itself, each element is represented by an array of DATA statements, with the chemical symbol used for the array name (which must be REAL type). Each array contains, in order, the atomic number Z^i, the mass number A^i, and the ionization potentials V_j^i, $j=1,2,\ldots, Z^i$. (Higher potentials which will not be needed in the calculation may be entered as zero.) In EIONX, /LMSB/ contains a single array name U, the contents of which are of course identical to those entered in MARI provided that the system loader uses MARI to define the COMMON block.

U(1), $Z^{(1)}$, charge number of first element
(2), $A^{(1)}$, mass number of first element
(3), $V_1^{(1)}$, first ionization potential of first element
:
$(Z^{(1)} + 2)$, $V_z^{(1)}$, last ionization potential of first element
$(Z^{(1)} + 3)$, $Z^{(2)}$, charge number of second element
etc.

/LMSC/M(51): Material definition and indexing information. M, Z and PART are equivalent array names.

M(1), NOLMNT, number of elements in the material. Note: INTEGER type.
Z(2), Z^i, charge number of first element in the material
PART(3), α_1, number fraction of atoms of first element in the material
M(4) index in the U array of the first entry (Z^i) for this element.
Z(5), $\bar{Z}^i$, mean ionic charge for this element
Z(6), $(\frac{\partial \bar{Z}^i}{\partial I})_\theta$
Z(7), $(\frac{J_i}{\theta} + \frac{3}{2})$
Z(8), J_i
Z(9), $(\frac{\partial \bar{Z}^i}{\partial \theta})_\tau$
Z(10), $(\frac{\partial \bar{Z}^i}{\partial \tau})_\theta$
Z(11), ε^i

} See Section 3.2.4 for definitions.

Z(12)
Z(51) } 10 word groups like Z(2)-Z(11) for up to 4 more elements

/LMSD/TLMS(30)

TLMS(1), BACK(1), $\bar{Z}^{(n)}$, previous iterate for $\bar{Z}$
(2), BACK(2), $\bar{Z}^{(n-1)}$, second previous iterate for $\bar{Z}$
(3) $\bar{A}$, mean atomic mass number
(4) temporary storage

(5) $\ln(\Gamma\bar{Z})$

(6), XBAR, X^i

(7), ZBARLN, $\ln \bar{Z}$

(8) temporary storage

(9), XI, $\varphi(\bar{N}^{-1} + \bar{Z})$

(10) $I = \theta \ln \Gamma$

(11) $\bar{Z}^{(n+1)} - 2\bar{Z}^{(n)} + \bar{Z}^{(n-1)}$ } terms for Aitken extrapolation

(12) $\bar{Z}^{(n+1)} - \bar{Z}^{(n)}$ }

(13) $V_j^i - V_{j-1}^i$

(14) $V_1^i + V_2^i + \cdots + V_{j-1}^i$

(15), DZDTAU $(\partial\bar{Z}/\partial\tau)_\theta$

(16), DZDTHT $(\partial\bar{Z}/\partial\theta)_\tau$

(17)-(30) temporary storage

/LMSE/: Internal flags, DO-loop indices, etc.

MATERL , material Identifier, from subroutine parameter M1

ILEMNT atomic charge number, U(I1)

SNAFU, PATH, internal error flag, special option flag

I1 index of Z in U array

I2 j, upper ionization stage index

I3 index of V_j^i in U array

I4

I5 iteration counter

I6

I7

I8, NJUMP

19, BYPASS, internal flow flag; INTEGER type

I10, M2

J1

J2, L0

J3

J4

J5

J6

/EOSIN/EIONIN(30): Specifies material composition for nonstandard materials.

Elements are in order of increasing Z.

EIONIN(1) (=NOLMNT), number of elements in this material; REAL type

(2), $Z^{(1)}$, atomic charge number of first element

(3), $\alpha^{(1)}$, number fraction of first element

(4), $Z^{(2)}$, atomic charge number of second element

.

.

.

(2*NOLMNT+1), Last entry for first material

. } up to 2 additional materials, specified as above.

(28), FESTER(1), option flag for molecular routines

(29), ZBRMIN(1), for $\bar{Z}$ less than this, ionization is ignored.

(30), EPSI(1), convergence criterion for $\bar{Z}$ iteration

/LMSG/CARBNZ(10): Communications area for carbon molecular routine CMOL. The first six words contain molecular contributions to energy, pressure, $(\partial E/\partial \tau)_\theta$, $(\partial E/\partial \theta)_\tau$, $(\partial P/\partial \tau)_\theta$, $(\partial P/\partial \theta)_\tau$, respectively.

/LMSESN/TLMSB(15): Communications and working storage for polyethylene molecular routine ESILMS. Words 12, 13, and 14 are equivalenced to DNDTAU, DNDTHT, and DISNRG, i.e., to $(\partial \bar{N}/\partial \tau)_\theta$, $(\partial \bar{N}/\partial \theta)_\tau$, and E_{dis} respectively.

3.6. MATERIAL IDENTIFICATION

The third subroutine parameter, M1, identifies the material according to the following list:

1-100 Single-element materials; M1=Z, the atomic charge number,

101	Polyethylene
102	Air
103	Teflon
104	Nylon-Phenolic A
105	Wet tuff
106	Refrasil
107	Phenolic A
108	Lithium Hydride
109	Salt
110	Magnalium
111	HMX
112	Refrasil B
113	Phenolic B
114	Refrasil C
115	Carbon-phenolic
116	First material specified in /EOSIN/
117	Second material specified in /EOSIN/
118	Third material specified in /EOSIN/
119-200	Currently invalid but reserved for multi-element material specifications
201-300	Reserved for equation-of-state routines not under control of EIONX
301-400	Reserved for special isotopic compositions of single-element materials; M1 = 300+Z

Care should be taken to use the multi-element version of EIONX if $100 < M1 \leq 200$. In other cases the single-element version is recommended. All elements called for in the M1 specification must be represented in the table of ionization potentials in /LMSB/.

3.7. OPTIONS

The fourth subroutine parameter, X3, may be used to specify a limited part of the entire EIONX procedure. X3=0. gives the complete calculation and is the normal setting. X^3=-1. provides for computing only

the two quantities

$$PHI = 9.648679 \times 10^{11} / \bar{A}$$

$$ZMEAN = \sum_i \alpha_i Z^i$$

X3=-2. suppresses all contributions from ionization by bypassing the $\bar{Z}$ calculation and setting $\bar{Z}=0$. X3=-3. is designed to provide communication with non-equilibrium ionic routines; the latter supply as input the following quantities in /LMSC/ for each element in the material:

M(10*i-6) Index in the U array of the first entry (Z^i) for the i^{th} element.

Z(10*i-5) $\bar{Z}^i$, mean ionic charge of i^{th} element.

Z(10*i-8) Z^i, charge number of i^{th} element.

The EIONX routine then evaluates the thermodynamic variables P, E, C_V, etc., and returns control to the calling routine. For M1=101, 6 or 306, this option should instead be specified by X3=-4., which allows for molecular contributions.

3.8. ERROR RETURNS

For sufficiently mild error conditions, a normal return is made at the completion of the calculation with a nonzero value of the parameter X3. For example, in the calculation of sound velocity the quantity

$$\frac{c_o^2}{\tau^2} = \frac{\theta}{C_V}\left(\frac{\partial P}{\partial \theta}\right)_\tau^2 - \left(\frac{\partial P}{\partial \tau}\right)_\theta$$

may turn out to be negative (this only occurs when ESILMS is used at very high densities). If so, the sound speed is set to zero and the above quantity is returned in X3. More serious errors cause an immediate return with the catastrophic error flag EION(14) set. The following list of EION(14) settings may be used for diagnostic purposes:

97.0097 Invalid M1 (material identifier)

97.0150 X1= $\theta <$ 0. or X2= $\tau < 10^{-30}$

97.0505 (Multi-element version): internal data statement altered incorrectly

97.0502 (Multi-element version): /EOSIN/data input (for M1=116, 117, or 118) incorrect

97.0012 (Multi version)
97.0003 (Single version)
} Needed element omitted from MARI

97.0607 (Multi version)
97.0007 (Single version)
} Needed ionization potential was zero.

97.0297 CMOL iteration did not converge.

97.0197 CMOL was called with $\tau < 0.1$

97.

3.9. APPENDIX: LISTING OF EIONX ROUTINES

```
BILT FOR  SINGLE
      SUBROUTINE EIONX  (X1, X2, M1, X3 )                                    M5  0020
C                                                                            M5  0030
C                                                                            M5  0040
C                                                                            M5  0050
C     CODED MAY,1965 BY LLW SCHALIT                                          M5  0060
C       RECODED ITERATION PROCEDURE FOR ZBAR MAY 6, 1966 BY G. LANE          M5  0070
C         LAST COMPILED BY G. LANE  JUNE 8,1966
C                                                                            M5  0080
C     *****      RATIONALE - THREE STAGE SAHA EQUATION ITERATIVE      *****M5  0100
C     *****                  SOLUTION.                                *****M5  0110
C                                                                            M5  0120
C     **********  CODED FOR SINGLE-ELEMENT-MATERIALS ONLY  **************M5  0130
C     **********  CODED FOR SINGLE-ELEMENT-MATERIALS ONLY  **************M5  0140
C     **********  CODED FOR SINGLE-ELEMENT-MATERIALS ONLY  **************M5  0150
C     **********  CODED FOR SINGLE-ELEMENT-MATERIALS ONLY  **************M5  0160
C     **********  CODED FOR SINGLE-ELEMENT-MATERIALS ONLY  **************M5  0170
C                                                                            M5  0180
C     ********** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS **********M5  0190
C     ********** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS **********M5  0200
C     ********** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS **********M5  0210
C     ********** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS **********M5  0220
C     ********** ZBAR .LE.1E-5 REVERTS TO PERFECT GAS ANSWERS **********M5  0230
C                                                                            M5  0240
C     EION(14) MUST BE NONZERO TO CALL A MOLLCULAR EQUATION OF STATE         M5  0250
C     EION(14) IS SET JUST BEFORE ENTRY TO THIS SUBROUTINE                   M5  0260
C                                                                            M5  0270
      COMMON/LMS/ EION(20)                                                   M5  0280
C                          VARIABLES  (INPUT AND OUTPUT)                     M5  0290
C                                                                            M5  0300
      REAL NBAR                                                              M5  0310
      EQUIVALENCE (EION(1),THETA),(EION(2),TAU),(EION(3),ZBAR)               M5  0320
      EQUIVALENCE (EION(4),ZBARI),(EION(5), PHI),(EION(6),ESHM)              M5  0330
      EQUIVALENCE (EION(7),PRESHR), (EION(8),ENERGY), (EION(9),DEDTHT)       M5  0340
      EQUIVALENCE(EION(10),DEDTAU),(EION(11),SNDSPD),(EION(12),DPDTAU)       M5  0350
      EQUIVALENCE (EION(13),DPDTHT)                                          M5  0360
      EQUIVALENCE(EION(16),ZMEAN),(EION(17),NBAR)                            M5  0370
C                                                                            M5  0380
C                                                                            M5  0390
      COMMON/LMSE/MATERL,ILEMNT,SNAFU,I1,I2,I3,I4,I5,I6,I7,I8,I9,I10,J1,    M5  0400
     2 J2,J3,J4,J5,J6                                                        M5  0410
      DATA MATERL,ILEMNT,SNAFU,I1,I2,I3,I4,I5,I6,I7,I8,I9,I10,J),            M5  0420
     2   J2,J3,J4,J5,J6/2*0.,0.,16*0/                                       M5  0430
      EQUIVALENCE (SNAFU,PATH)                                               M5  0440
      EQUIVALENCE (I8,NJUMP)                                                 M5  0450
      EQUIVALENCE (I10,M2)                                                   M5  0460
      EQUIVALENCE(L0,J2)                                                     M5  0470
      EQUIVALENCE (BFORE,J6)                                                 M5  0480
      INTEGER BYPASS                                                         M5  0490
      INTEGER BFORE                                                          M5  0500
C                                                                            M5  0510
C               MATERL IS INPUT AS M1                                        M5  0520
C                                                                            M5  0530
C     SNAFU IS THE INTERNAL SUBROUTINE ERROR FLAG CELL                       M5  0540
C     X3 IS SET TO SNAFU ON SUBROUTINE EXIT                                  M5  0550
C               X3 IS SET TO 0. IF NO SUBROUTINE ERRORS ARE FOUND            M5  0560
C                            TO BACK1 IF I5.GL.20 (THE ROUTINE USES THE      M5  0570
C               20TH ITERATE OF ZBARI AS ITS FINAL ANSWER.)                  M5  0580
C                                                                            M5  0590
C                          ABOVE ARE DO LOOP RUNNING INDICES OR JUMP NOS.    M5  0600
C               I1 SPECIFIES THE LOCATION OF THE ATOMIC NUMBER.              M5  0610
C               I2 SPECIFIES THE UPPER IONIZATION INDEX.                     M5  0620
C               I3 SPECIFIES THE LOCATION OF THE UPPER IONIZATION POTEN-     M5  0630
C                  TIAL.                                                     M5  0640
C               I5 COUNTS ITERATIONS                                         M5  0650
C                                                                            M5  0660
      COMMON/LMSD/          TLMS(30)                                         M5  0670
C                           TEMPORARY STORAGE                                M5  0680
```

```
C                                                                       M5  0690
      EQUIVALENCE(TLMS(1),BACT),(TLMS(2),[illegible]                    M5  0700
      EQUIVALENCE (XBAR,TLMS(6))                                        M5  0710
      EQUIVALENCE (TLMS(8),SIGMA ),(TLMS(9),XI )                        M5  0720
      EQUIVALENCE(TLMS(15),DZETAU )                                     M5  0730
      EQUIVALENCE(TLMS(16),DZLBIT)                                      M5  0740
      EQUIVALENCE(TLMS(27),XALFA1)                                      M5  0750
      EQUIVALENCE(TLMS(28),GAMMA)
      EQUIVALENCE(TLMS(29),CHI)
C                                                                       M5  0760
      COMMON/LMSC/ M(51)                                                M5  0770
      DIMENSION Z(51),PART(51)                                          M5  0780
C                                                                       M5  0790
      EQUIVALENCE(M(1),NOLMNT), (M(2),Z(2)),(M(3),PART(3))              M5  0800
C                                                                       M5  0810
C                                                                       M5  0820
      COMMON/LMSB/U(1)                                                  M5  0830
C                                                                       M5  0840
C                                                                       M5  0850
C                        ARRAY CONTAINING, FOR EACH ELEMENT, ATOMIC     M5  0860
C                        NUMBER, ATOMIC MASS, IONIZATION POTENTIALS IN  M5  0870
C                        INCREASING ORDER.                              M5  0880
C     *** THE ORDER (OF ELEMENTS IN THE TABLE) IS NOT SIGNIFICANT. FOR  M5  0890
C         HIGHEST SPEED, THOSE ELEMENTS MOST FREQUENTLY CALLED SHOULD BEM5  0900
C         PLACED FIRST.                                                 M5  0910
C                                                                       M5  0920
C               ARRAY FORMAT                                            M5  0930
C                  U(1) IS THE ATOMIC NUMBER OF THE FIRST ELEMENT,SAY ZAM5  0940
C                  U(2) IS ITS ATOMIC WEIGHT.                           M5  0950
C                  U(3),ETC. ARE,IN MONOTONE INCREASING ORDER,ITS ION-  M5  0960
C                       IZATION POTENTIALS. A MAXIMUM OF ZA SUCH ARE    M5  0970
C                       ALLOWED ARRAY ELEMENTS FROM U(3) THRU U(ZA+2).  M5  0980
C                       ALL IONIZATION POTENTIALS REQUIRED BY THE INPUT M5  0990
C                       THETA,TAU VALUES MUST BE LOADED. HIGHER POTEN-  M5  1000
C                       TIALS MAY BE INPUT AS ZERO OR MAY BE SKIPPED BY M5  1010
C                       THE INPUT DECK WITH A BSS CARD.                 M5  1020
C                  U(ZA+3) IS THE ATOMIC NUMBER OF THE SECOND ELEMENT,  M5  1030
C                       SAY ZB.                                         M5  1040
C                  U(ZA+4) IS THE ATOMIC WEIGHT OF THE SECOND ELEMENT.  M5  1050
C                  U(ZA+5) BEGINS ITS IONIZATION POTENTIAL TABLE.       M5  1060
C                                                                       M5  1070
C                                                                       M5  1080
      COMMON/LMSG/CARDNZ(10)                                            M5  1090
      COMMON/EOSIN/EIONIN(30)                                           M5  1100
      DIMENSION EPSI(1)                                                 M5  1110
      EQUIVALENCE(EPSI(1),EIONIN(30) )                                  M5  1120
      DATA EPSI/.001/                                                   M5  1130
      DIMENSION ZBRMIN(1)                                               M5  1140
      EQUIVALENCE(ZBRMIN(1),EIONIN(29) )                                M5  1150
      DATA ZBRMIN/.00001/                                               M5  1160
      DIMENSION  FESTER(1)                                              M5  1170
      EQUIVALENCE  (FESTER, EIONIN(28))                                 M5  1180
      DATA   FESTER/0./                                                 M5  1190
      DIMENSION ZLN(100)                                                M5  1200
C                                                                       M5  1210
C     EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.  M5  1220
C     OR IF A NEEDED IONIZATION POTENTIAL WAS FOUND TO BE ZERO          M5  1230
C     OR IF A NEEDED ELEMENT IS MISSING FROM THE MARI DECK              M5  1240
C     OR IF THETA(EV) WAS LESS THAN ZERO OR IF TAU(CC/G) WAS LESS THAN  M5  1250
C     1.E-30
C                                                                       M5  1270
      ENERGY=    0.                                                     M5  1280
      NBAR=      1.                                                     M5  1290
C                                                                       M5  1300
C                                                                       M5  1310
      PATH=      X3                                                     M5  1320
      THETA=     X1                                                     M5  1330
      TAU=       X2                                                     M5  1340
```

```
      IF(TAUTA.LT.0..OR.TAU.LT.1.E-30) GO TO 150
      IF(PATH.EQ.(-3.)) GO TO 6800                                          M5  1360
         IF (M1.GE.101.AND.M1.LE.300.OR.M1.GE.401.OR.M1.EQ.0) GO TO 97      M5  1370
         IF (M1 .EQ. M2 ) GO TO 91                                          M5  1380
      IF(PATH.EQ.-1.) GO TO 5033
      DO 503 I= 1,51
      Z(I)=     0.
      IF(I.GT.10) GO TO 503
      CARBNZ(I)= 0.
  503 CONTINUE
 5033 CONTINUE
      M2=       M1                                                          M5  1390
      ILEMNT=   M1                                                          M5  1400
C                                                                           M5  1410
         IF (ILEMNT.GE.301) GO TO 401                                       M5  1420
      IF(ILEMNT .EQ. 0) GO TO 97                                            M5  1430
      ISOTOP=    1                                                          M5  1440
  402 CONTINUE                                                              M5  1450
C                                                                           M5  1460
C                                                                           M5  1470
C                                                                           M5  1480
      II=        1                                                          M5  1490
      NJUMP=      1                                                         M5  1500
C                                                                           M5  1510
    2 J1=        U(II)                                                      M5  1520
      IF( J1-ILEMNT ) 3,52,3                                                M5  1530
C               FOR SHORTEST SEARCH, PUT IN ORDER OF MOST-NEEDED FIRST      M5  1540
C                                                                           M5  1550
C               AT EXIT, II= ARRAY LOCATION OF DESIRED Z=ATOMIC NO.         M5  1560
C               NEXT ARRAY ELEMENT IS THE ATOMIC WEIGHT. THIS IS FOLLOWED   M5  1570
C               BY THE SET OF IONIZATION POTENTIALS (MONOTONE INCREASING)   M5  1580
C                                                                           M5  1590
    3 CONTINUE                                                              M5  1600
      II=         II+J1+2                                                   M5  1610
      NJUMP=      NJUMP+1                                                   M5  1620
         IF (NJUMP .LT. 201 ) GO TO  2                                      M5  1630
      EION(14)=  97.0003                                                    M5  1640
      RETURN                                                                M5  1650
C     EION(14) IS SET IF A NEEDED ELEMENT HAS BEEN LEFT OUT OF THE          M5  1660
C     MAT1 DECK                                                             M5  1670
C                                                                           M5  1680
  401 CONTINUE                                                              M5  1690
      ISOTOP=    2                                                          M5  1700
      ILEMNT=    ILEMNT-300                                                 M5  1710
      GO TO 402                                                             M5  1720
  404 CONTINUE                                                              M5  1730
      ISOTOP=    1                                                          M5  1740
      GO TO 3                                                               M5  1750
C                                                                           M5  1760
   97 EION(14)= 97.0097                                                     M5  1770
      RETURN                                                                M5  1780
C     EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.      M5  1790
C                                                                           M5  1800
C                                                                           M5  1810
   52 CONTINUE                                                              M5  1820
         IF(ISOTOP.EQ.2) GO TO 404                                          M5  1830
      PHI=       9.648679E11 / U(II+1)                                      M5  1840
      M(1)=      1                                                          M5  1850
      Z(2)=      U(II)                                                      M5  1860
      PART(3)=   1.                                                         M5  1870
      M(4)=       II                                                        M5  1880
      ZMEAN=     U(II)                                                      M5  1890
      TLMS(3)=   U(II+1)                                                    M5  1900
C     THIS SECTION ALSO COMPUTES A MEAN ATOMIC NUMBER CALLED ZMEAN          M5  1910
   91 CONTINUE                                                              M5  1920
      IF(PATH .EQ. (-1.)) GO TO 1                                           M5  1930
C                                                                           M5  1940
      IF(PATH .EQ. (-2.)) GO TO 75                                          M5  1950
```

```
C
         IF (LION(14) .EQ. 0.) GO TO 599
C     LION(14) IS TO BE SET BEFORE ENTRY TO LIONEQ
C     LION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR FORM OF STATE
C     CARBON RUNS USING LIONX AND CMOL MUST SET LCHCK(J+17)    =.0050001)
         IF (ILEMNT .EQ. 6 ) CALL CMOL(TAU,THETA,FESTER)
C     FESTER IS LIONIN(28)
C     LIONIN(28) MUST BE SET .LT. 0. BY INPUT TO GET
C                TRANSLATION-ONLY CMOL
C     LIONIN(28) MUST BE SET .GT. 0. TO GET UBAR .EQ. 0. WHEN
C                T (DEG. KELVIN) .LT. 1500.
         IF (CARBNZ(8) .EQ. 0. ) GO TO 16
      LION(14)=  CARBNZ(8)
      RETURN
   16 CONTINUE
  599 CONTINUE
      IF(PATH.EQ.(-4.)) GO TO 6000
      TLMS(5)=  22.9926 + ALOG(TAU/PHI) + 1.5* ALOG(THETA)
C
      I5=         1
      IF((BFORE.GT.0).AND.(BFORE.LE.ILEMNT)) GO TO 1030
      IF(BFORE.GT.ILEMNT) GO TO 1010
C
      DO 1000 K=1,100
      AK=K
      AK=AK-.5
      ZLN(K)= ALOG(AK)
 1000 CONTINUE
C
 1010 CONTINUE
      J4=  ILEMNT
      J3=  ILEMNT/2
      J3=  MAX0(J3,1)
      IF(BFORE.EQ.0) J3= 1
      J5=  1
      GO TO 1050
C
 1030 CONTINUE
      TLMS(10)= THETA*(TLMS(5) -ZLN(BFORE))
      I3=         I1+1+BFORE
      I2=         BFORE
      IF(TLMS(10).LE. U(I3)) GO TO 1040
      IF(I2    .EQ.ILEMNT) GO TO 7
C
      J3=         BFORE +1
      J4=         ILEMNT
      J5=         1
      GO TO 1050
C
 1040 CONTINUE
      IF(I2.EQ.1) GO TO 14
      J3=         BFORE -1
      J4=         2*J3 -1
      J5=         2
C
 1050 CONTINUE
C
      DO 1060 K= J3,J4
      IF(J5.EQ.2) GO TO 1061
      I2=      K
      TLMS(10)= THETA*(TLMS(5) -ZLN(I2))
      I3=         I1 +1 +I2
      IF(TLMS(10).LE.U(I3)) GO TO 1070
C
 1060 CONTINUE
C
      IF(J5.EQ.2) GO TO 14
      GO TO 7
```

```
C                                                                       M5  2660
 1061 CONTINUE
      I2=         K- 2*(BFORE - I2)                                     M5  2540
      TLMS(10)= THETA*(TLMS(5) -ZLN(I2))                                M5  2560
      I3=         II+I2                                                 M5  2570
      IF(TLMS(10).GT.U(I3)) GO TO 1080
      GO TO 1060
C                                                                       M5  2600
 1070 CONTINUE                                                          M5  2670
      IF(I2.EQ.1) GO TO 14                                              M5  2680
      TLMS(10)= THETA*(TLMS(5) -ZLN(I2-1))
      BFORE=      I2                                                    M5  2690
      GO TO 1100                                                        M5  2700
C                                                                       M5  2710
 1080 CONTINUE                                                          M5  2720
      I2=         I2+1                                                  M5  2730
      I3=         I3+1                                                  M5  2740
      BFORE=      I2                                                    M5  2750
      GO TO 1100                                                        M5  2760
C                                                                       M5  2770
    7 CONTINUE                                                          M5  2780
        IF ( U(I3) .NE. 0. ) GO TO 601                                  M5  2790
      EION(14)=  97.0007                                                M5  2800
      RETURN                                                            M5  2810
C     EION(14) IS SET IF A NEEDED IONIZATION POTENTIAL WAS ZERO         M5  2820
C                                                                       M5  2830
  601 CONTINUE                                                          M5  2840
      I2=         ILEMNT                                                M5  2850
      BFORE=      I2                                                    M5  2860
      ZBAR1=      U(I1)                                                 M5  2870
      LO=         2                                                     M5  2880
      GO TO 9                                                           M5  2890
C                                                                       M5  2900
C                                                                       M5  2910
   14 CONTINUE                                                          M5  2920
      LO=         1                                                     M5  2930
      BFORE=      1                                                     M5  2940
C                                                                       M5  2950
    9 CONTINUE                                                          M5  2960
      TLMS(27)= EXP( TLMS(5)- U(I3)/THETA )                             M5  2970
      GO TO ( 93, 94) , LO                                              M5  2980
C                                                                       M5  2990
   93 CONTINUE                                                          M5  3000
      IF(ZBRMIN(1).LT.1.E-18) ZBRMIN(1)= 1.E-18                         M5  3010
        IF(TLMS(27).LE.(ZBRMIN(1)**2) ) GO TO  75                       M5  3020
C     ZBRMIN(1) IS THE MINIMUM ALLOWED ZBAR                             M5  3030
C                                                                       M5  3040
      ALPHA=   TLMS(27)                                                 M5  3050
   95 CONTINUE                                                          M5  3060
      XBAR=       .5* (-ALPHA+SQRT(ALPHA*ALPHA+4.*TLMS(27)))            M5  3070
      ZBAR1=   XBAR                                                     M5  3080
         IF (LO.EQ.2) ZBAR1 = ZBAR1 + U(I1) - 1.                        M5  3090
      IF(ZBAR1 .GT. ZMLAN) GO TO 98                                     M5  3100
      GO TO 13                                                          M5  3110
C                                                                       M5  3120
   94 CONTINUE                                                          M5  3130
      IF(TLMS(27).GT.1.E6) GO TO 13                                     M5  3140
      ALPHA=   TLMS(27)+U(I1) - 1.                                      M5  3150
      GO TO 95                                                          M5  3160
C                                                                       M5  3170
   75 CONTINUE                                                          M5  3180
C     PERFECT GAS PATH                                                  M5  3190
      SNAFU=    0.                                                      M5  3200
   99 CONTINUE                                                          M5  3210
      SIGMA=    0.                                                      M5  3220
      ZBAR1=    0.                                                      M5  3230
      ZBAR=     0.                                                      M5  3240
      GAMMA=    0.                                                      M5  3250
```

```
      CHI=        0.                                                    M5  3260
      XI=          PHI/NBAR                                             M5  3270
      LO=         4                                                     M5  3280
      GO TO 73                                                          M5  3290
C                                                                       M5  3300
   98 CONTINUE                                                          M5  3310
      SNAFU=      ZBAR1                                                 M5  3320
      GO TO 99                                                          M5  3330
C                                                                       M5  3340
 1100 CONTINUE                                                          M5  3350
      TLMS(4)=    I2                                                    M5  3360
      TLMS(13)= U(13)-U(13-1)                                           M5  3370
      TLMS(11)= TLMS(4) -1.5                                            M5  3380
      TLMS(12)= THETA/TLMS(3)                                           M5  3390
      TLMS(17)= TLMS(11) +(THETA*TLMS(5)-U(13-1))/TLMS(13)              M5  3400
      TLMS(19)= TLMS(17) -TLMS(12)*ZLN(I2-1)                            M5  3410
      TLMS(20)= 3.*TLMS(11) -TLMS(19) +2.*TLMS(12)                      M5  3420
      TLMS(21)= TLMS(11) -TLMS(19)                                      M5  3430
C                                                                       M5  3440
C                                                                       M5  3450
C                                                                       M5  3460
      BACK1=      0.                                                    M5  3500
      BACK2=      0.                                                    M5  3510
C                                                                       M5  3530
C                                                                       M5  3540
      XALFA1=     .5*(-TLMS(20) +SQRT(TLMS(20)*TLMS(20) -8.*TLMS(1))*   M5  3550
     2              TLMS(21))                                          M5  3560
C                                                                       M5  3570
      ZBAR1=      TLMS(11) +XALFA1                                      M5  3580
C                                                                       M5  3590
 1130 CONTINUE                                                          M5  3600
      IF(I5.GT.19) GO TO 1200                                           M5  3610
      BACK2=      BACK1                                                 M5  3620
      BACK1=      ZBAR1                                                 M5  3630
C                                                                       M5  3650
C                                                                       M5  3660
      TLMS(23)= XALFA1/(2.*TLMS(11) +XALFA1)                            M5  3670
      TLMS(24)= TLMS(23)*TLMS(23)                                       M5  3680
      TLMS(22)= .06666667*TLMS(12)*TLMS(23)*TLMS(24)                    M5  3690
      TLMS(25)= TLMS(22)*.6*TLMS(24)                                    M5  3700
      TLMS(26)=  .71428571*TLMS(24)*TLMS(25)                            M5  3710
C                                                                       M5  3720
      I5= I5+1                                                          M5  3730
      TLMS(18)= TLMS(22) +TLMS(25) +TLMS(26)                            M5  3740
C                                                                       M5  3750
      XALFA1=     (-TLMS(21)-TLMS(18))/(1.+TLMS(12)/(XALFA1+.5+TLMS(11))) M5  3760
      ZBAR1=      TLMS(11) +XALFA1                                      M5  3770
      IF(ABS(1.-BACK1/ZBAR1) -EPS1(1)) 1300,1300,1130                   M5  3780
C                                                                       M5  3790
 1200 CONTINUE                                                          M5  3800
      SNAFU=      BACK1                                                 M5  3810
      LO=         3                                                     M5  3815
      GO TO 600                                                         M5  3820
C                                                                       M5  3830
C                                                                       M5  3840
 1300 CONTINUE                                                          M5  3845
      LO=         3                                                     M5  3850
   13 CONTINUE                                                          M5  3860
      SNAFU=      0.                                                    M5  3870
  600 CONTINUE                                                          M5  3880
      ZBAR=       ZBAR1                                                 M5  3890
      XI=          (1./NBAR+ZBAR )*PHI                                  M5  3900
C                                                                       M5  3910
      GO TO (71,71,72),LO                                               M5  3920
   71 CONTINUE                                                          M5  3930
      GAMMA=      XBAR*ZBAR /(2.*XBAR+ALPHA)                            M5  3940
      IF(ZBAR.EQ.U(I1)) GAMMA= 0.                                       M5  3950
      IF(ZBAR.EQ.U(I1)) XBAR= 1.                                        M5  3960
```

```
      SIGMA=     XBAR  * U(13)*PHI                                    M5  3970
      CHI=       U(13) + 1.5 * THETA                                  M5  3980
      GO TO 73                                                        M5  3990
C                                                                     M5  4000
   72 CONTINUE
      TLMS(30)= TLMS(10) -TLMS(13)*(TLMS(18)+2.*TLMS(12)*TLMS(23))
      GAMMA=     THETA * ZBAR  / (THETA + ZBAR  * TLMS(13) )          M5  4010
      CHI=       TLMS(30)  +  1.5 * THETA                             M5  4020
      SIGMA=     ((ZBAR -TLMS(4)+1.5)**2)*TLMS(13)/2.*PHI             M5  4030
     2              + U(I3-1 ) * ( XI-TLMS(4)*PHI)                    M5  4040
C                                                                     M5  4050
C                                                                     M5  4060
   73 CONTINUE                                                        M5  4070
      Z(5)=      ZBAR                                                 M5  4080
C                                                                     M5  4090
      DZDTAU=    GAMMA / TAU                                          M5  4100
      DZDTHT=    GAMMA*CHI /THETA/THETA                               M5  4110
      PRESHR=    XI * THETA /TAU                                      M5  4120
      DPDTHT=    PRESHR/ THETA    +  PHI    *THETA/TAU * DZDTHT      M5  4130
      DPDTAU=    ( PHI     *THETA  *DZDTAU - PRESHR)/TAU              M5  4140
      DEDTAU=    PHI     *CHI * DZDTAU                                M5  4150
      DEDTHT=    XI * 1.5  +     PHI   * CHI   *DZDTHT                M5  4160
         IF (EION(14) .EQ. 0. ) GO TO 501                             M5  4170
C     EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR EQN OF STATE  M5  4180
C     EION(14) IS TO BE SET BEFORE ENTRY TO EIONEN                     M5  4190
      IF (ILEMNT.EQ.6) GO TO 500                                      M5  4200
  501 CONTINUE                                                        M5  4210
      SNDSPD=    TAU * SQRT (-DPDTAU + DPDTHT *DPDTHT * THETA /DEDTHT) M5  4220
C                                                                     M5  4230
      ENERGY=     ENERGY+XI*THETA*1.5+SIGMA                           M5  4240
      GO TO (100,77,77,100), LO                                       M5  4250
C                                                                     M5  4260
   77 TLMS(14)= 0.                                                    M5  4270
      I6=        I2 - 1                                               M5  4280
         IF (I6.EQ.0) GO TO 51
      DO 50 I4= 1, I6                                                 M5  4300
      J1= I1+I4+1                                                     M5  4310
      TLMS(14)= TLMS(14) +U(J1)                                       M5  4320
   50 CONTINUE                                                        M5  4330
   51 CONTINUE
C                                                                     M5  4340
C                                                                     M5  4350
      ENERGY=    ENERGY + TLMS(14)*PHI                                M5  4360
C                                                                     M5  4370
C                                                                     M5  4380
C                                                                     M5  4390
  100 CONTINUE                                                        M5  4400
      X3=        SNAFU                                                M5  4410
C                                                                     M5  4420
    1 CONTINUE                                                        M5  4430
C                                                                     M5  4440
      EION(14)=  0.                                                   M5  4450
      RETURN                                                          M5  4460
C                                                                     M5  4470
C                                                                     M5  4480
C                                                                     M5  4490
  150 CONTINUE                                                        M5  4500
      EION(14)=  97.0150                                              M5  4510
      RETURN                                                          M5  4520
C     SET EION(14) IF THETA.LT.ZERO OR TAU.LT. 1.E-30
C                                                                     M5  4540
  500 CONTINUE                                                        M5  4550
      ENERGY=    ENERGY+CARBNZ(1)                                     M5  4560
      DEDTAU=    DEDTAU+CARBNZ(3)                                     M5  4570
      DEDTHT=    DEDTHT+CARBNZ(4)                                     M5  4580
      DPDTAU=    DPDTAU+CARBNZ(5)                                     M5  4590
      DPDTHT=    DPDTHT+CARBNZ(6)                                     M5  4600
      GO TO 501                                                       M5  4610
```

```
C                                                                       M5  4620
C     ********************  PATH= -3.,-4.  ********************       M5  4630
 6000 CONTINUE                                                          M5  4640
C                                                                       M5  4650
      III=       M(4)                                                   M5  4660
      IF(Z(5).GT.(U(III)-.5)) GO TO 6010                                M5  4670
C                                                                       M5  4680
      GL=        Z(5)                                                   M5  4690
      LAG=       GL                                                     M5  4700
      GAL=     GL -FLOAT(LAG)                                           M5  4710
      IF(GAL.GT..5) II2= LAG +2                                         M5  4720
      IF(GAL.LE..5) II2= LAG +1                                         M5  4730
      GO TO 6020                                                        M5  4740
C                                                                       M5  4750
 6010 CONTINUE                                                          M5  4760
      II2=       Z(2)                                                   M5  4770
C                                                                       M5  4780
 6020 CONTINUE                                                          M5  4790
      II3=       III +II2 +1                                            M5  4800
C                                                                       M5  4810
      XI=        PHI*(1./ZBAR +ZBAR)                                    M5  4820
      IF(II2.EQ.1) GO TO 6030                                           M5  4830
      IF(II2.EQ.ILEMNT) GO TO 6040                                      M5  4840
C                                                                       M5  4850
      TLMS(4)=   II2                                                    M5  4860
      TLMS(13)= U(II3) -U(II3-1)                                        M5  4870
      SIGMA=     ((ZBAR  -TLMS(4) +1.5)**2)*TLMS(13)/2.*PHI +           M5  4880
     2              U(II3-1)*(XI -TLMS(4)*PHI)                         M5  4890
      GO TO 6060                                                        M5  4900
C                                                                       M5  4910
 6030 CONTINUE                                                          M5  4920
      XBAR=      ZBAR                                                   M5  4930
      GO TO 6050                                                        M5  4940
C                                                                       M5  4950
 6040 CONTINUE                                                          M5  4960
      XBAR=      ZBAR -U(III) +1.                                       M5  4970
C                                                                       M5  4980
 6050 CONTINUE                                                          M5  4990
      SIGMA=     XBAR*U(II3)*PHI                                        M5  5000
C                                                                       M5  5010
 6060 CONTINUE                                                          M5  5020
      PRESHR=    XI*THETA/TAU                                           M5  5030
      IF((PATH.EQ.(-4.)).AND.(ILEMNT.EQ.6)) ENERGY= ENERGY +CAPDIZ(1)   M5  5040
C                                                                       M5  5050
 6070 CONTINUE                                                          M5  5060
      ENERGY=    1.5*THETA*XI +SIGMA +ENERGY                            M5  5070
C                                                                       M5  5080
      TLMS(14)= 0.                                                      M5  5100
      IF(II2.EQ.1) GO TO 6080                                           M5  5090
      II6=       II2 -1                                                 M5  5110
      DO 6075 II4= 1,II6                                                M5  5120
      JJ1=       III +II4 +1                                            M5  5130
      TLMS(14)= TLMS(14) +U(JJ1)                                        M5  5140
 6075 CONTINUE                                                          M5  5150
 6080 CONTINUE                                                          M5  5160
C                                                                       M5  5170
      ENERGY=    ENERGY +TLMS(14)*PHI                                   M5  5180
C                                                                       M5  5190
      SNAFU=     0.                                                     M5  5200
      GO TO 100                                                         M5  5210
      CALL MARI
      RETURN
      END                                                               M5  5220
```

```
WILT FOR  MULTI
      SUBROUTINE EIONX  (X1, X2, M1, X3 )
C
C                                                                       0040
C                                                                       0050
C            CODED BY  LEW SCHALIT                                      0060
C     CODED DURING JUNE,1965                                            0070
C                                                                       0080
C          LAST COMPILED BY G. LANE  JUNE 8,1966                        0090
C
C     *****      RATIONALE - THREE STATE SAHA EQUATION ITERATIVE  *****  0110
C     *****                  SOLUTION.                            *****  0120
C     EION(14) MUST BE NONZERO TO CALL A MOLECULAR EQUATION OF STATE    0130
C     EION(14) IS SET JUST BEFORE ENTRY TO THIS SUBROUTINE              0140
C                                                                       0150
C     ********  ZBAR .LE. ZBRMIN REVERTS TO PERFECT GAS  ********       0160
C     ********  ZBAR .LE. ZBRMIN REVERTS TO PERFECT GAS  ********
C     ********  ZBAR .LE. ZBRMIN REVERTS TO PERFECT GAS  ********
C     ********  ZBAR .LE. ZBRMIN REVERTS TO PERFECT GAS  ********
C     ********  ZBAR .LE. ZBRMIN REVERTS TO PERFECT GAS  ********
C
C     ZBRMIN ORDINARILY SET .EQ. (.001) BUT MAY BE CHANGED BY INPUT
C     ZBRMIN ORDINARILY SET .EQ. (.001) BUT MAY BE CHANGED BY INPUT
C
C
C                                                                       0220
C                                                                       0230
      COMMON/LMS/ EION(20)                                              0240
C                                                                       0250
C                        VARIABLES  (INPUT AND OUTPUT)                  0260
      EQUIVALENCE (EION(1),THETA),(EION(2),TAU),(EION(3),ZBAR)          0270
      EQUIVALENCE (EION(4),ZBAR1),                (EION(6),ESUM)        0280
      EQUIVALENCE(EION(5),PHI)                                          0290
      EQUIVALENCE (EION(7),PRESHR), (EION(8),ENERGY), (EION(9),DEDTHT)  0300
      EQUIVALENCE(EION(10),DEDTAU),(EION(11),SNDSPD),(EION(12),DPDTAU)  0310
      EQUIVALENCE (EION(13),DPDTHT)                                     0320
      EQUIVALENCE(EION(16),ZMEAN)                                       0330
      EQUIVALENCE(EION(17),NBAR)                                        0350
      EQUIVALENCE (EION(18),ZSUM1),(EION(19),ZSUM2),(EION(20),ZSUM3)    0360
      REAL NBAR                                                         0370
C                                                                       0380
C                                                                       0390
C                                                                       0400
      COMMON/LMSD/          U(1)                                        0410
C                                                                       0420
C                           ARRAY CONTAINING, FOR EACH ELEMENT, ATOMIC  0430
C                           NUMBER, ATOMIC MASS, IONIZATION POTENTIALS IN 0440
C                           INCREASING ORDER.                           0450
C     *** THE ORDER (OF ELEMENTS IN THE TABLE) IS NOT SIGNIFICANT. FOR  0460
C         HIGHEST SPEED, THOSE ELEMENTS MOST FREQUENTLY CALLED SHOULD BE 0470
C         PLACED FIRST.                                                 0480
C                                                                       0490
C                 ARRAY FORMAT                                          0500
C                    U(1) IS THE ATOMIC NUMBER OF THE FIRST ELEMENT,SAY ZA 0510
C                    U(2) IS ITS ATOMIC WEIGHT.                         0520
C                    U(3),ETC. ARE,IN MONOTONE INCREASING ORDER,ITS ION- 0530
C                         IZATION POTENTIALS. A MAXIMUM OF ZA SUCH ARE  0540
C                         ALLOWED ARRAY ELEMENTS FROM U(3) THRU U(ZA+2). 0550
C                         ALL IONIZATION POTENTIALS REQUIRED BY THE INPUT 0560
C                         THETA,TAU VALUES MUST BE LOADED. HIGHER POTEN- 0570
C                         TIALS MAY BE INPUT AS ZERO.                   0580
C                    U(ZA+3) IS THE ATOMIC NUMBER OF THE SECOND ELEMENT, 0590
C                         SAY ZB.                                       0610
C                    U(ZA+4) IS THE ATOMIC WEIGHT OF THE SECOND ELEMENT. 0620
C                    U(ZA+5) BEGINS ITS IONIZATION POTENTIAL TABLE.      0630
C                                                                       0640
      COMMON/LMSC/ M(51)                                                0650
      DIMENSION Z(51),PART(51)                                          0660
                                                                        0670
```

```
C                                                                       0680
      EQUIVALENCE(M(1),NOLMNT), (EL(1),Z(1)),(C(1),FAC(1))              0690
C                                                                       0700
      COMMON/LMSD/          TLMS(30)
C                           TEMPORARY STORAGE                         0720
C                                                                       0730
      EQUIVALENCE(TLMS(1),BACK1),(TLMS(2),BACK2),(TLMS(7),ZBAR1D)       0740
      EQUIVALENCE(XBAR,TLMS(6))                                         0750
      EQUIVALENCE (TLMS(9),XI)                                          0760
      EQUIVALENCE(TLMS(15),DZETAU)                                      0770
      EQUIVALENCE(TLMS(16),DZETHT)                                      0780
C                                                                       0790
      COMMON/LMSE/MATERL,ILEMNT,SNAFU,I1,I2,I3,I4,I5,I6,I7,I8,I9,I10,I1, 0800
     2  J2,J3,J4,J5,J6
      EQUIVALENCE(L0,J2)
      DATA MATERL,ILEMNT,SNAFU,I1,I2,I3,I4,I5,I6,I7,I8,I9,I10,J1,J2,J3,
     2  J4,J5,J6/2*0.,16*0/
      EQUIVALENCE (SNAFU,PATH)                                          0810
      EQUIVALENCE (I8,NJUMP)                                            0820
      EQUIVALENCE (I9,BYPASS)                                           0830
      INTEGER BYPASS                                                    0840
      EQUIVALENCE (I10,M2)                                              0850
C                                                                       0860
C               MATERL IS INPUT AS M1                                   0870
C                                                                       0880
C     SNAFU IS THE INTERNAL SUBROUTINE ERROR FLAG CELL                  0890
C     I5 COUNTS ITERATIONS                                              0900
C     X3 IS SET TO SNAFU ON SUBROUTINE EXIT                             0910
C               X3 IS SET TO 0. IF NO SUBROUTINE ERRORS ARE FOUND       0920
C                     TO BACK1 IF I5.GE.20 (ROUTINE USES THE            0930
C               20TH ITERATE OF ZBAR1 AS ITS FINAL ANSWER. HOWEVER,THIS 0940
C               CASE MAY REQUIRE FURTHER INVESTIGATION, AS THE ITERATION0950
C               PROCEDURE MAY HAVE BEEN OSCILLATORY.)                   0960
C                                                                       0970
C                     ABOVE ARE DO LOOP RUNNING INDICES OR JUMP NOS.    0980
C               I1 SPECIFIES THE LOCATION OF THE ATOMIC NUMBER.         0990
C               I2 SPECIFIES THE UPPER IONIZATION INDEX.                1000
C               I3 SPECIFIES THE LOCATION OF THE UPPER IONIZATION POTEN-1010
C                  TIAL.                                                1020
C               I5 COUNTS ITERATIONS                                    1030
C                                                                       1040
      COMMON/LMSESN/TLMSB(15)                                           1050
      EQUIVALENCE(DNDTAU,TLMSB(12)),(DNDTHT,TLMSB(13))                  1060
      EQUIVALENCE(TLMSB(14),DISNRG)                                     1070
C                                                                       1080
      COMMON/LOSIN/EIONIN(30)
      DIMENSION EPSI(1)
      EQUIVALENCE(EPSI(1),EIONIN(30))
      DATA EPSI/.001/
      DIMENSION ZBRMIN(1)
      EQUIVALENCE(ZBRMIN(1),EIONIN(29))
      DATA ZBRMIN/.001/
      DIMENSION  FLSTER(1)
      EQUIVALENCE  (FESTER, EIONIN(28))
      DATA   FLSTER/0./
      COMMON/LMSG/CARDNZ(10)                                            1100
      DIMENSION    MATREL(11,15)
      REAL   MATREL
C
C     ARRAY FORMAT IS NO. OF ELEMENTS, SUCCESSIVE PAIRS OF
C           (ATOMIC NOS., ATOM NUMBER FRACTION) IN MONOTONI
C           INCREASING ORDER.  (FOR ENTRY CONVENIENCE ONLY)
C
      DIMENSION    DY1 (11), DY2 (11), DY3 (11), DY4 (11), DY5 (11),
     2             DY6 (11), DY7 (11), DY8 (11), DY9 (11), DY10(11),
     3             DY11(11), DY12(11), DY13(11), DY14(11), DY15(11)
C
      EQUIVALENCE  (MATREL(1,1), DY1(1))
```

```
      EQUIVALENCE  (MATREL(1,2), DY2(1))
      EQUIVALENCE  (MATREL(1,3), DY3(1))
      EQUIVALENCE  (MATREL(1,4), DY4(1))
      EQUIVALENCE  (MATREL(1,5), DY5(1))
      EQUIVALENCE  (MATREL(1,6), DY6(1))
      EQUIVALENCE  (MATREL(1,7), DY7(1))
      EQUIVALENCE  (MATREL(1,8), DY8(1))
      EQUIVALENCE  (MATREL(1,9), DY9(1))
      EQUIVALENCE  (MATREL(1,10), DY10(1))
      EQUIVALENCE  (MATREL(1,11), DY11(1))
      EQUIVALENCE  (MATREL(1,12), DY12(1))
      EQUIVALENCE  (MATREL(1,13), DY13(1))
      EQUIVALENCE  (MATREL(1,14), DY14(1))
      EQUIVALENCE  (MATREL(1,15), DY15(1))
C
C     ARRAY DY N IS FOR MATERL = (100+N)
C
C     **********MATERIAL CODE NUMBERS**********                              1820
C     CALL SEQUENCE PARAMETER L (RESET TO MATERL IN SUBROUTINE) IS           1830
C                  MATERL                  SUBSTANCE
C                    101                   POLYETHYLENE
C                    102                   AIR
C                    103                   TEFLON
C                    104                   NYLON-PHENOLIC A
C                    105                   WET TUFF
C                    106                   REFRASIL
C                    107                   PHENOLIC A
C                    108                   LITHIUM HYDRIDE
C                    109                   SALT
C                    110                   MAGNALIUM
C                    111                   H-M-X
C                    112                   REFRASIL B
C                    113                   PHENOLIC B
C                    114                   REFRASIL C
C                    115                   CARBON-PHENOLIC(R.SCHLAUG A)
C                    116                   CARD INPUT MATERIAL 1
C                    117                   CARD INPUT MATERIAL 2
C                    118                   CARD INPUT MATERIAL 3
C                                                                           2030
C
C     CH2
      DATA  DY1/2.,1., .666666667, 6., .333333333, 6*0./
C     AIR
      DATA  DY2/3.,7., .78455, 8., .21075, 18., .0047, 4*0./
C     TEFLON
      DATA  DY3/2.,6., .333333333, 19., .666666667, 6*0./
C     NYLON-PHENOLIC A
      DATA  DY4/4.,1., .5625, 6., .34375, 7., .03125, 8., .0625, 2*0./
C     WET TUFF
      DATA  DY5/5.,1., .310, 8., .497, 13., .033, 14., .137, 19., .023/
C     REFRASIL
      DATA  DY6/4.,1., .25, 6., .25, 8., .35, 14., .15, 2*0./
C     PHENOLIC A
      DATA  DY7/3.,1., .454545455, 6., .454545455, 8., .090909091, 4*0./
C     LITHIUM HYDRIDE
      DATA  DY8/2.,1., .5, 3., .5, 6*0./
C     SALT
      DATA  DY9/2.,11., .5, 17., .5, 6*0./
C     MAGNALIUM
      DATA  DY10/2.,12., .3, 13., .7, 6*0./
C     H-M-X
      DATA  DY11/4.,1., .285714285, 6., .142857142, 7., .285714285, 8.,
     2           .285714285, 2*0./
C     REFRASIL B
      DATA  DY12/4.,1., .19136, 6., .2392, 8., .39026, 14., .17918,2*0./
C     PHENOLIC B
      DATA  DY13/3.,1., .414, 6., .517, 8., .069, 4*0./
C     REFRASIL C
```

```
      DATA  DY14/5.,1.,  .248,  5.,  .007,  6.,  .292,  8.,  .321,  14.,  .132/
C     CARBON-PHENOLIC (R. SCHLAUG A)
      DATA  DY15/3.,1.,  .179,  6.,  .779,  8.,  .042,  4*0./
C
C
C                                                                              1110
C                                                                              1120
C                                                                              1130
C     EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.         1140
C     OR IF READ-IN INPUT IS INCORRECT
C     OR IF A MATERIAL DATA STATEMENT WAS ALTERED INCORRECTLY
C     OR IF A NEEDED IONIZATION POTENTIAL WAS FOUND TO BE ZERO                 1150
C     OR IF A NEEDED ELEMENT IS MISSING FROM THE MARI DECK                     1160
C     OR IF THETA(EV) WAS LESS THAN ZERO OR IF TAU(CC/G) WAS LESS THAN         1170
C     1.E-30
C                                                                              1190
C                                                                              1200
C                                                                              1250
C                                                                              1260
C                                                                              1270
C                                                                              1280
      PATH=      X3                                                            1290
      NBAR=      1.                                                            1300
      THETA=     X1                                                            1310
      TAU=       X2                                                            1320
      IF(THETA.LT.0..OR.TAU.LT.1.E-30) GO TO 150
      IF(PATH.EQ.(-3.)) GO TO 6000
      IF (M1 .EQ. M2 ) GO TO 91                                                1340
      DO 503 I= 1,51
      Z(I)=      0.
      IF(I.GT.15) GO TO 503
      TLMSB(I)=  0.                                                            1360
         IF (I .GT. 10 ) GO TO 503                                             1370
      CARBNZ(I)= 0.                                                            1380
  503 CONTINUE                                                                 1390
      MATERL=    M1                                                            1400
C                MATERL NAMES THE MATERIAL USED                                1410
      M2=        M1                                                            1420
C                                                                              1430
C                                                                              1440
C                                                                              1450
      IF(MATERL .LT. 101 ) GO TO 1                                             1460
C                ABOVE PATH FOR IONIC SINGLE ELEMENT MATERIAL                  1470
C                                                                              1480
      IF (MATERL .LT. 201) GO TO 2                                             1490
C                ABOVE PATH FOR IONIC MULTI-ELEMENT  MATERIAL                  1500
C                                                                              1510
         IF (MATERL .LT. 301 ) GO TO 97                                        1520
         IF (MATERL .LT. 401 ) GO TO 401                                       1530
C     MATERIAL NUMBERS FROM 301 TO 399 ARE TO BE USED FOR ISOTOPIC MIXES       1540
C     FOR SINGLE ELEMENT MATERIALS ONLY                                        1550
C     SUCH ISOTOPIC MIXES ARE TO BE ENTERED AFTER THE PURE ELEMENT ENTRY       1560
C     IF SUCH EXISTS                                                           1570
C                                                                              1580
   97 EION(14)= 97.0097                                                        1590
      RETURN                                                                   1600
C     EION(14) IS SET IF EIONX WAS CALLED WITH AN INVALID MATERIAL NO.         1610
C                                                                              1620
C                                                                              1630
    1 CONTINUE                                                                 1640
         IF (MATERL.EQ. 0) GO TO 97                                            1650
      ISOTOP=    1                                                            1660
      Z(2)=      MATERL                                                        1670
  402 CONTINUE                                                                 1680
C     THIS PATH FOR ANY SINGLE ELEMENT MATERIAL                                1690
      ILEMNT=    Z(2)                                                          1700
      NOLMNT=    1                                                             1710
      PART(3)=   1.                                                            1720
```

```
      GO TO 11                                                          1730
C                                                                       1740
  401 CONTINUE                                                          1750
      ISOTOP=    2                                                      1760
      Z(2)=      MATERL-300                                             1770
      GO TO 402                                                         1780
C                                                                       1790
    2 CONTINUE
      L = MATERL - 100
      ILEMNT=    0                                                      1810
      IF(L .GT. 15) GO TO 58
      SUMPRT = 0.
      NOLMNT = MATREL(1,L) + .5
      DO 10 I=1,NOLMNT
      MM = 2*I
      Z(10*I-8) = MATREL(MM,L)
      PART(10*I-7) = MATREL(MM+1,L)
      SUMPRT = SUMPRT + PART(10*I-7)
   10 CONTINUE
      IF(ABS(SUMPRT-1.) .LE. (.01)) GO TO 11
  505 CONTINUE
C     AN INTERNAL DATA STATEMENT FOR MATERIAL PROPERTIES
C        WAS ALTERED INCORRECTLY
      EION(14) = 97.0505
      RETURN
C
   58 CONTINUE                                                          4140
      IF(L .GT. 18) GO TO 97
      IF(L - 17) 581,59,60
C             PATH 58 FOR A FIRST MATERIAL USING READ-IN INPUT          4150
C             (INPUT TO BE ENTERED INTO THE EIONIN ARRAY IN             4160
C             FLOATING POINT FORM. NOLMNT TO BE ENTERED FIRST.          4170
C             THEN COME PAIRS OF ENTRIES FOR EACH ELEMENT OF            4180
C             ATOMIC NUMBER AND NUMBER FRACTION IN ORDER OF             4190
C             INCREASING ATOMIC NUMBER.  FURTHER MATERIALS STACK        4200
C             ON TOP.)                                                  4210
  581 MOPSY = 0
  504 CONTINUE                                                          4230
      SUMPRT = 0.
      NOLMNT = EIONIN(MOPSY+1) +.5                                      4240
         IF(NOLMNT .GT. 5.OR.NOLMNT.LE.0) GO TO 502                     4250
      DO 501 I=1,NOLMNT                                                 4260
      MOPSI=     2*I+MOPSY                                              4270
      Z(10*I-8)= EIONIN(MOPSI)                                          4280
      PART(10*I-7)=EIONIN(MOPSI+1)                                      4290
      SUMPRT = SUMPRT + PART(10*I-7)
  501 CONTINUE                                                          4300
      IF(ABS(SUMPRT-1.) .LE. (.01)) GO TO 11
C                                                                       4320
  502 CONTINUE                                                          4330
C     AN INPUT DATA WAS ENTERED INCORRECTLY
      EION(14) = 97.0502                                                4340
      RETURN
C                                                                       4360
   59 CONTINUE                                                          4370
C             PATH 59 FOR A SECOND MATERIAL USING READ-IN INPUT.        4380
C             SEE PATH 58 FOR INPUT INSTRUCTIONS.                       4390
      KRAZY = EIONIN(1) + .5                                            4400
      MOPSY=     2*KRAZY+1                                              4410
      GO TO 504                                                         4420
C                                                                       4430
   60 CONTINUE                                                          4440
C             PATH 60 FOR A THIRD MATERIAL USING READ-IN INPUT.         4450
C             SEE PATH 58 FOR INPUT INSTRUCTIONS.                       4460
      KRAZY=     EIONIN(1) + .5                                         4470
      KAT=       EIONIN(2*KRAZY+2) + .5                                 4480
      MOPSY=     2*(KRAZY+KAT+1)                                        4490
      GO TO 504                                                         4500
```

```
C                                                                       4510
C                                                                       4520
C                                                                       4530
C                                                                       4540
  404 CONTINUE                                                          4550
      ISOTOP=    1                                                    4560
      GO TO 403                                                        4570
C                                                                       4580
   11 CONTINUE                                                          4590
C                                                                       4600
C                                                                       4610
C     THE FOLLOWING SECTION INSERTS INTO THE 4TH,ETC., CELLS IN THE     4620
C     M ARRAY THE LOCATION INDEX FOR THE U ARRAY OF THAT ELEMENT WHOSE   4630
C     ATOMIC NUMBER WAS IN THE 2ND,ETC., CELL OF THE M ARRAY            4640
C     THE FACTOR   PHI   , WHICH IS A COMBINATION OF CONVERSION FACTORS, 4650
C     AND WEIGHTED ATOMIC MASSES, IS ALSO COMPUTED HERE                 4660
C     THIS SECTION ALSO COMPUTES A MEAN ATOMIC NUMBER CALLED ZMEAN      4670
C                                                                       4680
      TLMS(3)=  0.                                                     4690
      ZMEAN=     0.                                                    4700
      DO 14  I= 1, NOLMNT                                              4710
      I1=       1                                                      4720
      NJUMP=     1                                                     4730
   12 IF  (U(I1).EQ.Z(10*1-8) ) GO TO  13                              4740
  403 CONTINUE                                                          4750
      I1=       I1 + 2 + INT( U(I1) + .5 )                            4760
      NJUMP=     NJUMP+1                                              4770
         IF (NJUMP .LT. 201 ) GO TO 12                                 4780
      EION(14)=  97.0012                                               4790
      RETURN                                                           4800
C     EION(14) IS SET IF A NELDED ELEMENT HAS BEEN LEFT OUT OF THE      4810
C     MART DECK                                                         4820
   13 CONTINUE                                                          4830
         IF ( ISOTOP .EQ. 2 ) GO TO 404                                4840
      ZMEAN=     ZMEAN+PART(10*I-7)*U(I1)                              4850
      M(10*I-6)=I1                                                     4860
      TLMS(3)=  TLMS(3)+  PART(10*I-7) * U(I1+1)                       4870
C     TLMS(3) IS THE MEAN PARTICLE WEIGHT                               4880
   14 CONTINUE                                                          4890
      PHI=       9.648679E11/TLMS(3)                                   4900
C                                                                       4910
C                                                                       4920
   91 CONTINUE                                                          4930
C                                                                       4940
         IF (PATH .EQ.(-1.) ) GO TO 100                                4950
C                                                                       4960
C
         IF((MATERL.EQ.6.OR.MATERL.EQ.306).AND.EION(14).NE.0.)CALL CMOL
     1(TAU,THETA,FESTER)
C     FESTER IS EIONIN(28)
C     EIONIN(28) MUST BE SET .LT. 0. BY INPUT TO GET
C                TRANSLATION-ONLY CMOL
C     EIONIN(28) MUST BE SET .GT. 0. TO GET NOAR .EQ. 9. WHEN
C                T (DEG. KELVIN) .LT. 1500.
C     EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR EQN OF STATE   4980
C     CARBON RUNS USING EIONX AND CMOL MUST SET ECHCK(J+17) = 5.98566E11
         IF (CARBNZ(8) .EQ. 0. ) GO TO 16                               4990
      EION(14)=  CARBNZ(8)                                             5000
      RETURN                                                           5010
C     EION(14) IS TO BE SET BEFORE ENTRY TO EIONFN                      5020
C                                                                       5030
C                                                                       5040
   16 CONTINUE                                                          5050
C                                                                       5060
      IF ( MATERL.NE.102) GO TO 700                                    5070
      IF ( THETA .GT. EION(14) ) GO TO 700                             5080
C     IF THETA.LE.EION(14) (WHICH WAS SET BEFORE ENTRY TO EIONFN) RETURN 5090
C     TO A MOLECULAR AIR EQUATION OF STATE                              5100
```

```
C     EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR ION OF STATE          5110
C     EION(14) IS TO BE SET BEFORE ENTRY TO EIONEN                             5120
C     AIR RUNS USING EIONEN AND AIR13 MUST SET ECHCK(J+17) TO AIR
C         DISSOCIATION ENERGY (ABOUT 2.9E11)
      MATERL=    208                                                         5130
      GO TO 100                                                              5140
  700 CONTINUE                                                               5150
C                                                                            5160
C                                                                            5170
      IF(MATERL.NE.101) GO TO 92                                             5180
C     EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR ION OF STATE         5190
C     EION(14) IS TO BE SET BEFORE ENTRY TO EIONEN                           5200
C     THE ESILMS SUBROUTINE IS CALLED WHENEVER THE MOLECULAR SPECIES         5210
C        CHARACTERISTIC OF CH2 DECOMPOSITION ARE BELIEVED PRESENT.           5220
      TLMSB(1)= .78+.20833*ALOG(TAU)                                         5230
C     CH2 RUNS USING ESILMS AND EIONE3 MUST HAVE ECHCK(J+17) = 9.63E))       5240
      IF (THETA.LT..207107+1./TLMSB(1).AND. EION(14) .NE. 0.)CALL ESILMS     5250
C                                                                            5260
   92 CONTINUE                                                               5300
C                                                                            5310
         IF (PATH.EQ.(-2.)) GO TO 90                                         5320
C                                                                            5330
      IF(PATH.EQ.(-4.)) GO TO 6000
C                                                                            5290
      DO 93 I=1,NOLMNT                                                       5340
      Z(10*I)=  0.                                                           5350
   93 CONTINUE                                                               5360
C                                                                            5370
C                                                                            5380
C                                                                            5390
C                                                                            5400
C     WHEN ABOVE DO LOOP FINISHES,M(1) =NOLMNT                               5410
C                                                                            5420
C                                  M(2) =            Z OF FIRST ELEMENT      5430
C                                  M(12)=            Z OF 2ND ELEMENT        5440
C                                  M(22)=            Z OF 3RD ELEMENT        5450
C                                  M(32)=            Z OF 4TH ELEMENT        5460
C                                  M(42)=            Z OF 5TH ELEMENT        5470
C                                                                            5480
C                                  M(3) =NUMBER FRACTION OF 1ST ELEMENT      5490
C                                  M(13)=NUMBER FRACTION OF 2ND ELEMENT      5500
C                                  M(23)=NUMBER FRACTION OF 3RD ELEMENT      5510
C                                  M(33)=NUMBER FRACTION OF 4TH ELEMENT      5520
C                                  M(43)=NUMBER FRACTION OF 5TH ELEMENT      5530
C                                                                            5540
C                                  M(4) =LOCATION OF Z OF FIRST ELEMENT      5550
C                                  M(14)=LOCATION OF Z OF 2ND ELEMENT        5560
C                                  M(24)=LOCATION OF Z OF 3RD ELEMENT        5570
C                                  M(34)=LOCATION OF Z OF 4TH ELEMENT        5580
C                                  M(44)=LOCATION OF Z OF 5TH ELEMENT        5590
C                                                                            5600
C                                                                            5610
C     THE VALUE OF ZBAR FOR EACH SPECIES PRESENT IS STORED IN THE 5TH,       5620
C              ETC., ARRAY ELEMENTS AFTER IT IS COMPUTED.                    5630
C                                                                            5640
      ZSUM1=    0.                                                         5650
      ZSUM2=    1.                                                         5660
      ZSUM3=    0.                                                         5670
      ZBAR=     0.                                                         5680
      ZBARLN=   0.                                                         5690
      BACK1=    0.                                                         5700
      I5=       1                                                          5710
      BYPASS=   0                                                          5720
C             SETS ITERATION COUNTER                                         5730
C                                                                            5740
      TLMS(5)=  ALOG(TAU/PHI)+1.5*ALOG(THETA)+22.9926                      5750
   21 CONTINUE
      TLMS(10)= THETA*(TLMS(5)-ZBARLN)
```

```
C                TLMS(10) IS THE SYNTHETIC POTENTIAL USED IN EQUATIONS          5770
   22 DO 23 I=1,NOLMNT                                                          5780
C                                                                               5790
C                                                                               5800
C                                                                               5810
C                                                                               5820
      I1=        M(10*I-6)                                                     5830
      ILEMNT=    U(I1) + .5                                                    5840
C                                                                               5850
C                AT ENTRY,I1= ARRAY LOCATION OF DESIRED Z=ATOMIC NO.           5860
C                IN THE U(250) ARRAY                                           5870
C                NEXT ARRAY ELEMENT IS THE ATOMIC WEIGHT. THIS IS FOLLOWE      5880
C                BY THE SET OF IONIZATION POTENTIALS (MONOTONE INCREASNG)       5890
C                                                                               5900
C                                                                               5910
      DO 607 I2=1,ILEMNT                                                        5920
      I3=        I2+I1+1                                                       5930
      IF (TLMS(10).LE.U(I3)) GO TO 608                                          5940
  607 CONTINUE                                                                  5950
         IF ( U(I3) .NE. 0.) GO TO 601                                          5960
      LION(14)=  97.0607                                                        5970
      RETURN                                                                    5980
C     EION(14) IS SET IF A NEEDED IONIZATION POTENTIAL WAS ZERO                 5990
  601 CONTINUE                                                                  6000
      I2=        ILEMNT                                                        6010
C                                                                               6020
      IF ( I5 .EQ. I ) BACK1 = U(I1)                                            6030
      LO=        2                                                             6040
      GO TO 609                                                                 6050
C                                                                               6060
C                                                                               6070
C                                                                               6080
  608 CONTINUE                                                                  6090
      IF (I2.EQ.1) GO TO 614                                                    6100
C                                                                               6110
C                                                                               6120
  620 TLMS(13)= U(I3)-U(I3-1)                                                   6130
      TLMS(4)=   I2                                                             6140
      LO=        3                                                             6150
      ZBAR1=     TLMS(4) - 1.5 + (TLMS(10)-U(I3-1) ) / TLMS(13)                 6160
      GO TO 641                                                                 6170
C                                                                               6180
C                                                                               6190
   95 CONTINUE                                                                  6200
      IF ( NOLMNT .EQ. 1 ) BACK1 = 1.E-20                                       6210
      XBAR=      1.E-20                                                         6220
      ZBAR1=     1.E-20                                                         6230
      IF ( NOLMNT .EQ. 1 ) GO TO 90                                             6240
      GO TO 641                                                                 6250
C                                                                               6260
   96 CONTINUE                                                                  6270
      XBAR=      1.                                                             6280
      ZBAR1=     U(I1)                                                          6290
      GO TO 641                                                                 6300
C                                                                               6310
  614 CONTINUE                                                                  6320
      LO=        1                                                             6330
C                                                                               6340
  609 CONTINUE                                                                  6350
      I4=        10*I                                                          6360
      IF ( Z( I4 ).EQ.0.) Z( I4 )= EXP(TLMS(5)-U(I3)/THETA)                     6370
      ZBRLOW=     (ZBRMIN(1)*.1)**2
      IF(ZBRLOW.EQ.0.) ZBRLOW= 1.E-38
C     ZBRMIN(1) IS THE MINIMUM ALLOWED ZBAR
      IF (Z(I4).LT.ZBRLOW.AND.LO.EQ.I) GO TO 95
      IF (Z(I4).GT.(1.E6).AND.LO.EQ.2) GO TO 96
      IF (I5.EQ.1 .AND. LO.EQ.I) BACK1= SQRT (.5*Z(                             6400
      XBAR=      Z(I4)/(Z(I4)+BACK1)                                            6410
```

```
      ZBAR1=    XBAR                                                        6420
      IF (12.NE.1)   ZBAR1= ZBAR1 * U(I1)-1.                                6430
  641 CONTINUE                                                              6440
C                                                                           6450
      I6=       10*1-7                                                    6460
C     16 IS PART INDEX                                                    6470
C                                                                           6480
      ZBAR=     ZBAR+ PART(I6) * ZBAR1                                    6490
C                                                                           6500
C                                                                           6510
C                                                                           6520
C                                                                           6530
C                                                                           6540
      IF (BYPASS.EQ.0) GO TO 23                                           6550
C                                                                           6560
      ESUM=     0.                                                        6570
      IF (12.EQ.1) GO TO 664                                              6580
      I7=       I2-1                                                      6590
      DO 660 J1=1,17                                                      6600
      I8=       J1+I1+1                                                   6610
      ESUM=     ESUM +U(18)                                               6620
  660 CONTINUE                                                            6630
  664 CONTINUE                                                            6640
C                                                                           6650
C                                                                           6660
C                                                                           6670
      Z(10*1-5)=ZBAR1                                                     6680
C                                                                           6690
C     EQUIVALENCE(M(1),Z(1))                                              6700
C                                    M(5) = 1ST ELEMENT MEAN IONIC CHARGE   6710
C                                    M(15)= 2ND ELEMENT MEAN IONIC CHARGE   6720
C                                    M(25)= 3RD ELEMENT MEAN IONIC CHARGE   6730
C                                    M(35)= 4TH ELEMENT MEAN IONIC CHARGE   6740
C                                    M(45)= 5TH ELEMENT MEAN IONIC CHARGE   6750
C                                                                           6760
C                                                                           6770
      GO TO (650,650,651),LO                                              6780
  650 CONTINUE                                                            6790
      TLMS(4)=  XBAR-XBAR*XBAR                                            6800
      Z(10*I-4)=TLMS(4)/THETA                                             6810
      Z(10*1-3)=U(13)/THETA+1.5                                           6820
      Z(10*I-2)=U(13)                                                     6830
      Z(10*1+1)=XBAR *U(13)                                               6840
      ZSUM1=    ZSUM1+PART(I6)*Z(10*I-4)*Z(10*1-3)                        6850
      ZSUM2=    ZSUM2+PART(I6)*XBAR/(Z(I4)  +BACK1)                       6860
      ZSUM3=    ZSUM3+PART(16) * TLMS(4)/TAU                              6870
      GO TO 653                                                           6880
  651 CONTINUE                                                            6890
      Z(10*I-4)=1./TLMS(13)                                               6900
      Z(10*1-3)=TLMS(10)/THETA +1.5                                       6910
      Z(10*1-2)=TLMS(10)                                                  6920
      Z(10*I+1)=U(I3-1)*(ZBAR1-TLMS(4)+1.)+.5* TLMS(13)      *(ZBAR1-     6930
     2            TLMS(4)+1.5)**2                                         6940
      ZSUM1=    ZSUM1+PART(16)*Z(10*1-3)/TLMS(13)                         6950
      ZSUM2=    ZSUM2+ PART(I6) /  TLMS(13) *THETA /BACK1                 6960
      ZSUM3=    ZSUM3+ PART(16)/ TLMS(13)*THETA/TAU                       6970
  653 CONTINUE                                                            6980
      Z(10*1+1)=ESUM+Z(10*1+1)                                            6990
   23 CONTINUE                                                            7000
      IF(ZBAR .GT. ZMEAN) GO TO 94
C                                                                           7010
C                                                                           7020
      IF ( ABS(1.- BACK1/ZBAR)-EPS1(1).LE. 0.) BYPASS= 1+BYPASS           7030
      IF(BYPASS .GE. 2) GO TO 41
   30 CONTINUE                                                            7050
      IF ( I5 .GT. 2 ) GO TO 40                                           7060
   31 BACK2=    BACK1                                                     7070
      BACK1=    ZBAR                                                      7080
```

```
      I5=       I5+I                                                    7090
      ZBARLN=   ALOG(ZBAR)                                              7100
      ZBAR=     0.                                                      7110
      GO TO 21                                                          7120
C                                                                       7130
C                                                                       7140
   32 CONTINUE
      SNAFU=    ZBAR
      BYPASS=   2
      GO TO 31
C                                                                       7170
   40 CONTINUE                                                          7180
         IF(ZBAR.LT.ZBRMIN(1) ) GO TO 90
C     ZBRMIN(I) IS THE MINIMUM ALLOWED ZBAR
C     EXIT IF ZBAR IS TOO SMALL
      TLMS(11)= ZBAR -2.* BACK1 + BACK2                                 7210
      HOLDZ=    ZBAR                                                    7220
      TLMS(12)= ZBAR -BACK1                                             7230
      ZBAR=     ZBAR -(TLMS(12)**2) / TLMS(11)                          7240
C     ABOVE IS AITKENS DEL-SQUARE ITERATION CONVERGENCE IMPROVEMENT     7250
C     PROCEDURE                                                         7260
         IF((ZBAR.LE.0.).OR.(ZBAR.GT.ZMEAN)) ZBAR=.5*(HOLDZ+BACK1)
      IF(I5 .GT. 18) GO TO 32
      GO TO 31                                                          7290
C                                                                       7300
   94 CONTINUE
      SNAFU=    ZBAR
      GO TO 98
C                                                                       7310
   90 CONTINUE                                                          7320
C     PERFECT GAS PATH                                                  7330
      SNAFU=    0.                                                      7380
   98 CONTINUE
      LO=        4
      ZBAR=     0.                                                      7340
      XI=        PHI/NBAR                                               7350
      DZDTHT=   0.                                                      7360
      DZDTAU=   0.                                                      7370
      GO TO 43                                                          7390
C                                                                       7400
  101 CONTINUE                                                          7410
      IF (THETA.GE..207107+1./TLMSH(1)) GO TO 80                        7420
C                                                                       7430
C     LOW TEMPERATURE POLYETHYLENE PATH                                 7440
      ENERGY=   ENERGY + DISNRG * (TLMSB(4)-1.)                         7450
      DEDTHT=   DEDTHT + DNDTHT*THETA* 1.5 *PHI + DISNRG *TLMSB(11)     7460
      DEDTAU=   DEDTAU + DNDTAU*THETA* 1.5 *PHI+DISNRG*TLMSB(10)        7470
      DPDTHT=   DPDTHT + DNDTHT*THETA/ TAU*PHI                          7480
      DPDTAU=   DPDTAU + DNDTAU*THETA/ TAU*PHI                          7490
      GO TO 80                                                          7500
  500 CONTINUE                                                          7510
      ENERGY=    ENERGY+CARBNZ(1)                                       7520
      DEDTAU=    DEDTAU+CARBNZ(3)                                       7530
      DEDTHT=    DEDTHT+CARBNZ(4)                                       7540
      DPDTAU=    DPDTAU+CARBNZ(5)                                       7550
      DPDTHT=    DPDTHT+CARBNZ(6)                                       7560
      GO TO 80                                                          7570
C                                                                       7580
C                                                                       7590
   41 CONTINUE                                                          7600
         IF(ZBAR.LT.ZBRMIN(1) ) GO TO 90
C     ZBRMIN(I) IS THE MINIMUM ALLOWED ZBAR
C     EXIT IF ZBAR IS TOO SMALL
   42 CONTINUE                                                          7630
      DZDTHT=   ZSUM1/ZSUM2                                             7640
      DZDTAU=   ZSUM3/ZSUM2                                             7650
      XI=        PHI*(I./NBAR+ZBAR)                                     7660
   43 CONTINUE                                                          7670
```

```
      PRESHR=    XI*THETA/TAU                                              7680
      DPDTHT=    PRESHR/THETA + THETA/TAU*DZDTHT + PHI                     7690
      DPDTAU=    ( THETA*PHI*DZDTAU-PRESHR ) / TAU                         7700
      ENERGY=    1.5*XI*THETA                                              7710
      DEDTHT=    1.5*(XI*THETA*DZDTHT + PHI)                               7720
      DEDTAU=    1.5*THETA*DZDTAU*PHI                                      7730
         IF ( EION(14) .EQ. 0. ) GO TO 80                                  7740
C     EION(14) IS TO BE SET BEFORE ENTRY TO EIONEQ                         7750
C     EION(14) MUST BE SET NONZERO TO CALL THE MOLECULAR EQN OF STATE      7760
         IF (MATERL.EQ.6.OR.MATERL.EQ.306) GO TO 500                       7770
      IF (MATERL.EQ.101) GO TO 101                                         7780
   80 CONTINUE                                                             7790
      IF(ZBAR .EQ. 0.) GO TO 669                                           7800
      DO 662 I= 1,NOLMNT                                                   7810
      I6=        10*I-7                                                    7820
C     I6 INDEXES PART ARRAY                                                7830
      Z(10*I-1)=Z(10*I-4)* ( Z(10*I-3) -THETA/ZBAR*DZDTHT)                 7840
      Z(10*I)=   Z(10*I-4) *THETA * ( 1./TAU - DZDTAU/ZBAR)                7850
      ENERGY=    ENERGY+PART(I6)*PHI*Z(10*I+1)                             7860
      DEDTHT=    DEDTHT+PART(I6)*PHI*Z(10*I-2)*Z(10*I-1)                   7870
      DEDTAU=    DEDTAU+PART(I6)*PHI*Z(10*I-2)*Z(10*I)                     7880
  662 CONTINUE                                                             7890
  669 CONTINUE                                                             7900
      ARGSQ=     -DPDTAU +DPDTHT*DPDTHT*THETA/DEDTHT
      IF(ARGSQ.GT.0.) GO TO 1669
      IF(SNAFU.EQ.0.) SNAFU= ARGSQ
      ARGSQ=     0.
 1669 CONTINUE
      SNDSPD=    TAU*SQRT(ARGSQ)
C                                                                          7920
  670 CONTINUE
      X3=        SNAFU                                                     7930
  100 CONTINUE                                                             7940
      EION(14)=  0.                                                        7950
C                                                                          7960
C                                                                          7970
      RETURN                                                               7980
C                                                                          7990
  150 CONTINUE                                                             8000
      EION(14)=  97.0150                                                   8010
      RETURN                                                               8020
C     SET EION(14) IF THETA.LT.ZERO OR TAU.LT. 1.E-30
C                                                                          8040
C
C*********************  SPECIAL PATH  ********************
C********************* PATH=  -3.  ***********************
C
 6000 CONTINUE
      DO 6010 II= 1,NOLMNT
      III=       M(10*II-6)
C
      IF(Z(10*II-5).GT.(U(III)-.5)) GO TO 6005
      GL=        Z(10*II-5)
      LAG=       GL
      GAL=       GL -FLOAT(LAG)
      IF(GAL.GT..5) II2= LAG +2
      IF(GAL.LE..5) II2= LAG +1
      GO TO 6007
 6005 CONTINUE
      II2=       Z(10*II-8)
C
 6007 CONTINUE
      II3=       II2 +III +1
C
      ESUM=      0.
      IF(II2.EQ.1) GO TO 6060
      II7=       II2 -1
      DO 6050 JJ1= 1,II7
```

```
      II8=       JJ1 +III +1
      ESUM=      ESUM +U(II8)
 6050 CONTINUE
 6060 CONTINUE
      IF(Z(10*II-5).LE..5) GO TO 6100
      IF(Z(10*II-5).GT.(U(III)     -.5)) GO TO 6110
      GO TO 6130
C
 6100 CONTINUE
      XBAR=      Z(10*II-5)
      GO TO 6120
 6110 CONTINUE
      XBAR=      Z(10*II-5) -U(III) +1.
 6120 CONTINUE
      Z(10*II+1)= XBAR*U(II3)
      GO TO 6140
 6130 CONTINUE
      ZBAR1=     Z(10*II-5)
      TLMS(4)=   FLOAT(II2)
      TLMS(13)= U(II3) -U(II3-1)
      Z(10*II+1)= U(II3-1)*(ZBAR1 -TLMS(4) +1.) +.5*TLMS(13)*(ZBAR1 -
     2              TLMS(4) +1.5)**2
 6140 CONTINUE
      Z(10*II+1)= Z(10*II+1) +ESUM
 6010 CONTINUE
C
C
 6143 CONTINUE
      XI=        PHI*(1./NBAR +ZBAR)
C
      PRESHR=    XI*THETA/TAU
C
      ENERGY=    1.5*XI*THETA
C
      IF(PATH.EQ.(-3.)) GO TO 6150
      IF(MATERL.EQ.6.OR.MATERL.EQ.306) ENERGY= ENERGY +CARBNZ(1)
      IF(MATERL.EQ.101) GO TO 6200
 6150 CONTINUE
      DO 6160 II= 1,NOLMNT
      II6=       10*II-7
      ENERGY=    ENERGY +PART(II6)*PHI*Z(10*II+1)
 6160 CONTINUE
C
      SNAFU=     0.
      GO TO 670
 6200 CONTINUE
      IF(THETA.GE..207107+1./TLMSB(1)) GO TO 6150
      ENERGY=    ENERGY +DISNRG*(TLMSB(4)-1.)
      GO TO 6150
      CALL MARI
      RETURN                                                          8050
      END
```

SECTION IV

EQUATION OF STATE INVERSION FROM TEMPERATURE-DENSITY TO SPECIFIC ENERGY-DENSITY BY TABLE LOOK-UP

4.1. INTRODUCTION

In order to obtain solutions to the general equations for inviscid, compressible fluid flow with radiation and/or conduction energy transport mechanisms, it is necessary to specify at least the following thermodynamic variables: pressure, P; temperature, θ ; specific internal energy, E; and density, ρ . The equations which relate these four thermodynamic quantities are usually referred to as the equations of state. If local thermodynamic equilibrium (LTE) is assumed, the equations for the thermodynamic variables can be completely specified by only two independent variables (e.g., temperature and density).

Some computer programs use equations of state with θ and ρ as the independent variables and others use E and ρ . Comparison of problems calculated using both types of programs can be extremely difficult unless completely consistent representations are used. The inversion of an equation of state given in terms of the temperature and density to the (E, ρ) form is thus required. For many materials of interest, analytic inversion from (θ, ρ) to (E, ρ) is not a trivial matter.

4.2. METHOD

One method of inverting equations of state from (θ , ρ) space to (E, ρ) space is to use a table look-up procedure to interpolate from one set of variables to the other. In the scheme reported here a two step process is used to obtain the necessary conversion. First, a table is generated from data given (or calculated) with θ and ρ as independent variables. This

table is punched on cards in DATA STATEMENT form. Second, these DATA STATEMENTS become part of a code which can be used as a subroutine to determine the temperature and pressure given E, and ρ or $\tau = 1/\rho$.

The actual values of θ and P are not tabulated. Instead, the table entries have been chosen to be $\bar{Z}$, the mean number of free electrons per atom, and $\ell n\, I$ where I is the internal energy due to ionization and excitation. The quantities $\bar{Z}$ and $\ell n\, I$ are both rather weak functions of density and energy over most of their range, which gives rise to a minimum error when interpolating between table entries.

The other thermodynamic variables are easily expressed in terms $\bar{Z}$ and I. In addition, other material properties, such as absorption coefficients, can be conveniently calculated from $\bar{Z}$.

The method of preparing the tables of $\bar{Z}$ and $\ell n\, I$ is fairly straightforward. The range of E and τ is determined by available data or as needed for a particular application. The tabular entries are picked such that

$$E_m = E_Z \cdot 10^{(m-1)/T}$$

$$\tau_n = \tau_Z \cdot 10^{(n-1)/S}$$

where E_Z = minimum value of E,

τ_Z = minimum value of τ,

T = desired number of points per decade for E,

S = desired number of points per decade for τ.

The values of $\bar{Z}$ and $\ell n\, I$ at the desired value of E and τ are obtained from the existing (θ, ρ) equation of state. If interpolation is required, the energy is forced to be within 0.1% of the desired value. The values of τ and E at each point do not have to be saved.

For any arbitrary pair of values of (E, τ), the proper region on the table can easily be calculated. Let

$$N = (\log_{10} (\tau / \tau_Z) * S + 1)$$

and

$$M = (\log_{10} (E/E_Z) * T + 1) \qquad (103)$$

and let

n = truncated value of N

and

m = truncated value of M. (104)

Entries at (n, m), (n, m + 1), (n + 1, m), and (n + 1, m + 1) can then be used to obtain interpolated values for $\overline{Z}$ and $\ell n\, I$ at the desired value of (E, τ).

4.3. PROGRAM GEST

The program GEST generates a table of $\overline{Z}$ and $\ell n\, I$ for the values of E, τ specified by input data. If the minimum value of E is specified as zero by the input data, then the program will calculate E_Z as $E_Z(\theta_o, \tau_{max})$, where τ_{max} is specified by input and θ_o is chosen such that

$$\overline{Z}\ (\theta_o,\ \tau_{max}) < \frac{0.2\theta_o}{V_1}$$

where V_1 is the first ionization potential of the given material.

To generate this table, an interpolation must be performed between an initial guess at a temperature θ' which will produce E' and an unknown temperature θ which will produce the desired value of E indicated by the input data. Newton's method of linear interpolation is used repeatedly until a relative error of 0.1% is obtained between successive interpolations. Then the values of $\overline{Z}$ and I are obtained using the final value of θ. If I is found to be less than 10^{-10} ev, then I is set equal to 10^{-10} ev. The

process is repeated for each value of E and τ specified. Once the table of $\bar{Z}$ and $\ell n\ I$ is generated, the DATA STATEMENTS for the program EST are punched. (NOTE: For punching DATA STATEMENTS on an IBM-7044, the IBM FORTRAN IV print and punch routine ECV must be used.)

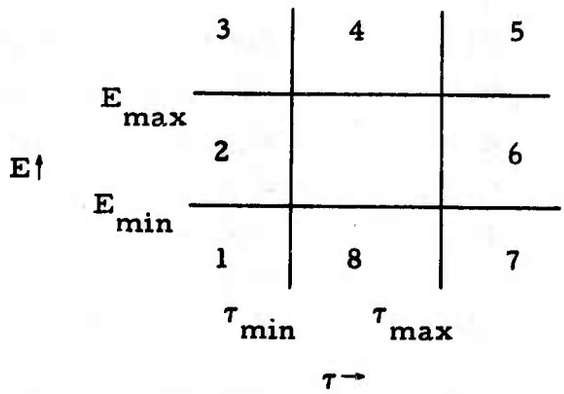
4.3.1. Input

Cards 1 and 2 have a floating point field width of 10, and card 3 had an integer field width of 5.

	Mnemonic	Comment
Card 1	Z	Atomic number
	A	Atomic mass number
	V1	First ionization potential
	VZ	Last ionization potential
	S	Number of tabular pts./decade of τ
	T	Number of tabular pts./decade of E
	DN	Number of decades of τ
Card 2	DM	Number of decades of E
	TAUZ	Min. value of τ in table
	EZ	Min. value of E in table. If zero, program will calculate an EZ.
Card 3	IS	Source of information used to generate table. (NOTE: At this writing an IS of 1 indicating the use of EIONX (see Section III) is the only option available.)

	Mnemonic	Comment
Card 3 (Continued)	I1 → I8	Flags to indicate the use of a special treatment at the boundaries of the table. If the flag is a 1, the calculation will stop when the region is entered. If zero, the calculation will proceed with the available analytic equation in the general EOS program.

Regions of the table as defined by I1 through I8:



4.3.2. Output

The output appears in two forms: printed output (for checking input data and the calculations of the table), and punched card output. The punched cards are in DATA STATEMENT form for immediate placement into the program EST, which performs further equation of state calculations from this data.

4.4. PROGRAM EST

The program EST performs a two-dimensional linear interpolation within the limits of the table supplied it by the program GEST. If a region is entered which is outside the limits of the table, the calculation will either stop or go to an analytic solution which is based on the values of the table at the boundary.

Within the limits of the table, Eqs. (103) and (104) are used to find indices (as functions of E and τ) for use in an interpolation formula to find $\bar{Z}$ and $\ell n\, I$. The interpolation formula used is as follows:

$$\bar{Z}(E,\tau) = \bar{Z}_{n,m} + (\bar{Z}_{n+1,m} - \bar{Z}_{n,m})\, D1 + (\bar{Z}_{n,m+1} - \bar{Z}_{n,m})\, D2$$

$$+ (\bar{Z}_{n+1,m+1} + \bar{Z}_{n,m} - \bar{Z}_{n+1,m} - \bar{Z}_{n,m+1})\, D1 \times D2 \qquad (105)$$

where

$$D1 = N - n \text{ and } D2 = M - m \qquad (106)$$

The interpolation used to obtain $\ell n\, I$ is performed in the same manner as for $\bar{Z}$ by replacing $\bar{Z}$ with $\ell n\, I$ in Eq. (105). The quantity I is then evaluated as $\exp(\ell n\, I)$.

At this writing only regions 7 and 8 referred to in Section 4.3.1 have been supplied with analytic solutions. These solutions are based on using a crude approximation to the Saha equation. For $\theta \gg I$ the value of $\bar{Z}^2$ is proportional to

$$\tau\theta^{3/2}\, e^{-V_1/\theta} \qquad (107)$$

where V_1 is the first ionization potential of the material being described. Therefore, given $\bar{Z}(E_o, \tau_o)$ from the table boundary, where $E_o = E_Z$,

$$\left(\frac{\bar{Z}(E,\tau)}{\bar{Z}(E_o,\tau_o)}\right)^2 = \left(\frac{\theta'}{\theta_o}\right)^{3/2} \left(\frac{\tau}{\tau_o}\right) \exp\left[\left(\frac{1}{\theta_o} - \frac{1}{\theta'}\right) V_1\right] \qquad (108)$$

In both regions 7 and 8, θ' is set to $(E/E_Z)\theta_o$. In region 8, $\tau = \tau_o$, $\theta_o = f(E_Z, \tau)$, and Eq. (108) can be written

$$\bar{Z}(E,\tau) = \bar{Z}(E_Z,\tau) \left(\frac{\theta'}{\theta_o}\right)^{3/4} \exp\left[\left(\frac{1}{\theta_o} - \frac{1}{\theta'}\right) \frac{V_1}{2}\right] \qquad (109)$$

For region 7, $\tau_o = \tau_{max}$ on the boundary of the table, $\theta_o = f(E_Z, \tau_{max})$, and Eq. (108) is written

$$\bar{Z}(E, \tau) = \bar{Z}(E_Z, \tau_{max}) \left(\frac{\tau}{\tau_{max}}\right)^{1/2} \left(\frac{\theta'}{\theta_o}\right)^{3/4} \exp\left[\left(\frac{1}{\theta_o} - \frac{1}{\theta'}\right) \frac{V_1}{2}\right] \quad (110)$$

For both regions 7 and 8, the value for I is approximated as $\bar{Z}$ times V_1.

The temperature and pressure are obtained, given $\bar{Z}$ and I, from the relations

$$\theta = (E/\varphi - I) / \left| 1.5(1 + \bar{Z}) \right| \quad (111)$$

where

$$\varphi = 9.648679 \times 10^{11}/A$$

$$P = \varphi (1 + \bar{Z}) \theta/\tau$$

Section 4.5 contains the mnemonics used for both GEST and EST. Section 4.6 contains a listing of GEST and EST and an error routine, ERR, used by GEST. EST also includes a list of the DATA STATEMENTS produced by the program GEST. E, τ, and P are in cgs units, and θ and I are in ev.

4.5. APPENDIX: MNEMONICS FOR GEST AND EST

A	*
AIN	I, in ev
ALGE	$\log_{10} E$
ALGT	$\log_{10} \tau$
ALIN	$\ell n\, I$
DLGE	$\log_{10} (E/E_0)$
DLGT	$\log_{10} (\tau/\tau_0)$
DMLE	ΔE above position n, m in table
DNLT	$\Delta\tau$ above position n, m in table
E	Specific internal energy
EILN1D	Array of $\ell n\, I$
EL	$\log_{10} E$

*See input for GEST

EM	Max value of E for table
EMAX	Value of E used in interpolation
EMIN	Value of E used in interpolation
EZ	*
I	Ionization energy
I1-I8	*
IS	*
M	Index for table entries
N	Index for table entries
PHI	φ (see Eq. (111))
T	*
τ	Specific volume
TAUL	$\log_{10} \tau$
TAUM	Max value of τ for table
TAUZ	*
THETA	θ (temperature in ev)
THMAX	θ max used in interpolation
THMIN	θ min used in interpolation
V1	*
VF	*
Z	*
ZBAR	$\bar{Z}$, mean number of free electrons
ZBID	Array of ZBAR

*See input for GEST

4.6. APPENDIX: LISTING OF GEST AND EST

```
@I    FOR   GEST/A, GEST/RSE1, GEST/R1
C     GENERATE EQUATION OF STATE TABLES
C
      DIMENSION    THETA(50,50),CARD(14)
      DIMENSION    TAUL(50),TAU(50),EL(50),E(50),ZB1D(2500),EILN1D(2500)
      COMMON/LMS/ EION(20)
      COMMON/LMSD/         TLMS(16)
      EXPT(Q)=EXP(2.3026*Q)
    1 FORMAT  (12A6)
      READ (5,1)  (CARD(I), I = 1, 12)
      WRITE (6,1)  (CARD(I), I = 1, 12)
 9000 FORMAT (7F10.5)
 9001 FORMAT(14I5)
 9002 FORMAT(1X,1P7E10.4)
 9003 FORMAT(6X14H DIMENSION ZB(I2,1H,I2,7H),EILN(I2,1H,I2,1H))
 9004 FORMAT(6X35H EQUIVALENCE (ZB,ZB1), (EILN,EILN1) )
 9005 FORMAT(5XI1,6(1P1E10.3,1H,))
 9006 FORMAT(6X24H DATA TAULZ,EZ,Z,S,T,PHI/ )
 9007 FORMAT(6X36H DATA NN,MM,I1,I2,I3,I4,I5,I6,I7,I8/ )
 9008 FORMAT(5XI1,1H/)
 9009 FORMAT(6X16HCOMMON/EST/EILN(I2,1H) )
 9010 FORMAT (4H  EL)
 9011 FORMAT (6H  TAUL)
 9012 FORMAT (6H  ZBAR)
 9013 FORMAT (7H  THETA)
 9014 FORMAT(5XI1,1P1E10.3,5(1H,1P1E10.3),1H/)
 9015 FORMAT(6X,8H DATA ZBI2,1H/)
 9016 FORMAT(6X14H COMMON/EST/ZBI2,1H(I2,1H) )
 9017 FORMAT(6H  EILN)
 9018 FORMAT(6X28H DATA TAUM,EM,TAUZ,EZ,V1,VZ/)
 9019 FORMAT(5XI1,9(I3,1H,),I3,1H/)
 9020 FORMAT(6X11H DATA EILN/)
 9021 FORMAT(6X10H DATA EILNI2,1H/)
 9022 FORMAT(6X16H COMMON/EST/EILNI2,1H(I2,1H) )
 9031 FORMAT(5XI1,1P1E10.3,1H/)
 9032 FORMAT(5XI1,1P1E10.3,  1H,1P1E10.3 ,1H/)
 9033 FORMAT(5XI1,1P1E10.3,2(1H,1P1E10.3),1H/)
 9034 FORMAT(5XI1,1P1E10.3,3(1H,1P1E10.3),1H/)
 9035 FORMAT(5XI1,1P1E10.3,4(1H,1P1E10.3),1H/)
 9036 FORMAT(5XI1,1P1E10.3,5(1H,1P1E10.3),1H/)
C        READ AND STORE INPUT
      READ(5,9000) Z,A,V1,VZ,S,T,DN,DM,TAUZ,EZ
      WRITE(6,9002) Z,A,V1,VZ,S,T,DN,DM,TAUZ,EZ
      READ(5,9001) IS,I1,I2,I3,I4,I5,I6,I7,I8
      WRITE(6,9001)IS,I1,I2,I3,I4,I5,I6,I7,I8
C        Z = ATOMIC CHARGE NO.
C        A = ATOMIC MASS NO.
C       V1 = FIRST IONIZATION POTENTIAL
C       VZ = LAST IONIZATION POTENTIAL
C        S = NO. OF TABULAR PTS/DECADE OF TAU
C        T = NO. OF TABULAR PTS/DECADE OF E
C       DN = NO. OF DECADES OF TAU
C       DM = NO OF DECADES OF E
C     TAUZ = MIN VALUE OF TAU IN TABLE
C       EZ = MIN VALUE OF  E  IN TABLE
C       IS = SOURCE USED FOR TABLE GENERATION
C          = 1 USE EIONX
C       I1 THRU I8 FLAGS INDICATING TREATMENT AT BOUNDARIES OF TABLE
C       IN = 1 STOP IF REGION IS ENTERED
C          = 0 CALCULATE WITH AVAILABLE ANALYTIC EQS
C        3 * 4 * 5
C        *********
C          *   *
C     E 2 *   * 6
C          *   *
C        *********
```

```
C       1 * 8 * 7
C         TAU
        L=Z
        PHI=9.648679L11/A
        AM=T*DM+1.0
        AN=S*DN+1.0
        NN=AN
        MM=AM
        TAUM=TAUZ*10.0**DN
        TAUL(1)=ALOG10(TAUZ)
        DTAUL=1./S
        TAU(1) = TAUZ
        IF(EZ. NE.0.) GO TO 30
        THA = 1.1
        DO 20  I=1,10
   10   THA = THA - .1
        CALL EIONX(THA,TAUM,L,0.)
        S1 = EION(14)
        IF(S1.NE.0.) CALL ERR(S1)
        IF(EION(3).GT. .2 * THA/V1) GO TO 20
        EZ = EION(8)
        GO TO 30
   20   CONTINUE
        S1 = 10.20
        CALL ERR(S1)
   30   CONTINUE
C         PREPARE TABLES OF SPECIFIC DENSITY AND ENERGY
C         IN REAL SPACE AND IN LOG BASE 10.
        DO 50 I=2,NN
        TAUL(I)=TAUL(I-1)+DTAUL
        TAU(I)=EXPT(TAUL(I))
   50   CONTINUE
        EM=EZ*10.0**DM
        EL(1)=ALOG10(EZ)
        DEL=1./T
        E(1) = EZ
        DO 60 I=2,MM
        EL(I)=EL(I-1)+DEL
        E(I)=EXPT(EL(I))
   60   CONTINUE
        WRITE (6,9011)
        WRITE (6,9002) (TAUL(N), N = 1,NN)
        WRITE (6,9010)
        WRITE (6,9002) (EL(M), M = 1,MM)
C         DETERMINE SOURCE OF EOS DATA
        GO TO (100,200,300,400),IS
  100   CONTINUE
        DO 149 M=1,MM
        DO 149 N=1,NN
        K=(M-1)*NN+N
C         INITIAL GUESS AT THE TEMPERATURE
        THMIN = THETA(N,M-1)
        THMAX = THETA(N-1,M)
        IF(N.EQ.1) THMAX=E(M)/PHI
        IF( (N.EQ.1).AND.(M.GT.1) ) THMAX=3.*THETA(N,M-1)
        IF(M.EQ.1) THMIN =1.E-3
        THETA(N,M) =THMIN
        DO 120 I=1,20
        CALL EIONX(THMIN,TAU(N),L,0.)
        S1=EION(14)
        IF(S1.NE.0.) CALL ERR(S1)
        EMIN=EION(8)
        CALL EIONX(THMAX,TAU(N),L,0.)
        EMAX=EION(8)
        S1=EION(14)
```

```
      IF(S1.NE.0.) CALL ERR(S1)
      CALL EIONX(THETA(N,M),TAU(N),L,0.)
C        NEWTON'S INTERPOLATION
      THETA(N,M)=THETA(N,M)+(THMAX-THMIN)*(E(M)-EION(8))
     1           /(EMAX-EMIN)
      IF(ABS(EION(8)-E(M))  /E(M).LE..001) GO TO 130
      IF(EION(8).LT.E(M)) THMIN=THETA(N,M)
      IF(EION(8).GT.E(M)) THMAX=THETA(N,M)
  120 CONTINUE
      S1=10.120
      CALL ERR(S1)
  130 CONTINUE
C        ZBAR AND EION OBTAINED FROM EIONX
      ZB1D(K)=EION(3)
      AEI=(EION(8)-1.5*EION(1)*TLMS(9))/PHI
      IF( AEI.LE. 1.E-10) AEI=1.E-10
      EILN1D(K) =ALOG(AEI)
  149 CONTINUE
C        RESERVED FOR FUTURE SOURCES OF EOS DATA
  200 CONTINUE
  300 CONTINUE
  400 CONTINUE
C
C        PUNCH DATA STATEMENTS FOR PROGRAM EST
  500 CONTINUE
      ID=1
      PUNCH 9018
      PUNCH 9036,ID,TAUM,EM,TAUZ,EZ,V1,VZ
      PUNCH 9006
      PUNCH 9035,ID,TAUL(1),EL(1),S,T,PHI
      PUNCH 9007
      PUNCH 9019,ID,NN,MM,I1,I2,I3,I4,I5,I6,I7,I8
      PUNCH 9003,NN,MM,NN,MM
      PUNCH 9004
      KM=NN*MM
      NM=KM
      IF(NN*MM.GT.54) NM=54
      PUNCH 9016,ID,NM
      PUNCH 9015,ID
      ICNT=0
      DO 549 I=1,KM,6
      I6=I+5
      ICNT=ICNT+1
      IP=I
      IF((I6.LT.KM).OR.(ICNT.EQ.10) ) GO TO 539
  530 I6=KM
      KI=KM-I+1
      GO TO (531,532,533,534,535),KI
  531 PUNCH 9031,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
  532 PUNCH 9032,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
  533 PUNCH 9033,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
  534 PUNCH 9034,ICNT,(ZB1D(K),K=IP,I6)
      GO TO 548
  535 PUNCH 9035,ICNT,(ZB1D(K),K=IP,I6  )
      GO TO 548
  539 IF(ICNT.LT.10) GO TO 540
      ID=ID+1
      NM=54
      IF((ID  )*54.GT.KM) NM=KM-(ID-1)*54
      PUNCH 9016,ID,NM
      PUNCH 9015,ID
      ICNT=1
```

```
      IF(I6.GT.KM) GO TO 530
      GO TO 545
  540 IF(ICNT.NE.9) GO TO 545
      PUNCH 9036,ICNT,(ZB1D(K),K=I,I6)
      GO TO 548
  545 PUNCH 9005,ICNT,(ZB1D(K),K=I,I6)
  548 CONTINUE
  549 CONTINUE
      NM=KM
      IF(NN*MM.GT.54) NM=54
      ID=1
      PUNCH 9022,ID,NM
      PUNCH 9021,ID
      ICNT =0
      DO 599 I=1,KM,6
      I6=I+5
      ICNT=ICNT+1
      IP=I
      IF((I6.LT.KM).OR.(ICNT.EQ.10) ) GO TO 570
  560 I6=KM
      KI=KM-I+1
      GO TO (561,562,563,564,565),KI
  561 PUNCH 9031,ICNT,(EILN1D(K),K=IP,I6)
      GO TO 598
  562 PUNCH 9032,ICNT,(EILN1D(K),K=IP,I6)
      GO TO 598
  563 PUNCH 9033,ICNT,(EILN1D(K),K=IP,I6)
      GO TO 598
  564 PUNCH 9034,ICNT,(EILN1D(K),K=IP,I6)
      GO TO 598
  565 PUNCH 9035,ICNT,(EILN1D(K),K=IP,I6)
      GO TO 598
  570 IF(ICNT.LT.10) GO TO 580
      ID=ID+1
      NM=54
      IF((ID  )*54.GT.KM) NM=KM-(ID-1)*54
      PUNCH 9022,ID,NM
      PUNCH 9021,ID
      ICNT=1
      IF(I6.GT.KM) GO TO 560
      GO TO 585
  580 IF(ICNT.NE.9) GO TO 585
      PUNCH 9036,ICNT,(EILN1D(K),K=I,I6)
      GO TO 598
  585 PUNCH 9005,ICNT,(EILN1D(K),K=I,I6)
  598 CONTINUE
  599 CONTINUE
C         EDIT PRINTS
  600 CONTINUE
      WRITE (6,9012)
      WRITE(6,9002) (ZB1D(K),K=1,KM)
      WRITE(6,9017)
      WRITE(6,9002) (EILN1D(K),K=1,KM)
      WRITE (6,9013)
      WRITE (6,9002) ((THETA(N,M), N = 1,NN), M = 1,MM)
  700 CONTINUE
      CALL EXIT
      END
@I    FOR   ERR/A, ERR/RSE1, ERR/R1
       SUBROUTINE ERR(S1)
    3 FORMAT (6H S1 = F10.4)
      WRITE(6,3) S1
      CALL EXIT
      END
@I    FOR  LIBEX, LIBEX/FJ
```

```
      SUBROUTINE LIBEX(TAU,E,THA,P,ZBAR,GG)
      COMMON Z(90)
      EQUIVALENCE (Z(90),S1)
C*****PLACE DATA STATEMENTS PRODUCED BY PROGRAM GEST HERE  ******
      DATA TAUM,EM,TAUZ,EZ,V1,VZ/
     1 5.000E+10, 1.583E+12, 5.000E-02, 1.583E+09, 7.980E+00, 1.126E+03/
      DATA TAULZ,ELZ,S,T,PHI/
     1 -1.301E+0,  9.2,        2.000E+0,  8.000E+0,  5.244E+9/
      DATA NN,MM,I1,I2,I3,I4,I5,I6,I7,I8/
     1 25, 25,  1,  1,  1,  1,  1,  1,  0,  0/
      DIMENSION ZB(25,25),EILN(25,25)
      EQUIVALENCE (ZB,ZB1), (EILN,EILN1)
      COMMON/EST/ZB 1(54)
      DATA ZB 1/
     1 2.200E-10, 3.912E-10, 6.957E-10, 1.237E-09, 2.200E-09, 3.912E-09,
     2 6.957E-09, 1.237E-08, 2.200E-08, 3.912E-08, 6.957E-08, 1.237E-07,
     3 2.200E-07, 3.911E-07, 6.955E-07, 1.236E-06, 2.197E-06, 3.904E-06,
     4 6.930E-06, 1.229E-05, 2.173E-05, 3.828E-05, 6.694E-05, 1.156E-04,
     5 1.957E-04, 3.911E-08, 6.956E-08, 1.237E-07, 2.200E-07, 3.911E-07,
     6 6.955E-07, 1.237E-06, 2.198E-06, 3.907E-06, 6.941E-06, 1.232E-05,
     7 2.184E-05, 3.863E-05, 6.803E-05, 1.189E-04, 2.054E-04, 3.475E-04,
     8 5.694E-04, 9.132E-04, 1.382E-03, 1.984E-03, 2.722E-03, 3.553E-03,
     9 4.455E-03, 5.399E-03, 2.001E-06, 3.563E-06, 6.333E-06, 1.125E-05/
      COMMON/EST/ZB 2(54)
      DATA ZB 2/
     1 1.997E-05, 3.542E-05, 6.265E-05, 1.104E-04, 1.932E-04, 3.342E-04,
     2 5.669E-04, 9.331E-04, 1.499E-03, 2.279E-03, 3.284E-03, 4.485E-03,
     3 5.898E-03, 7.394E-03, 8.953E-03, 1.054E-02, 1.217E-02, 1.375E-02,
     4 1.529E-02, 1.679E-02, 1.823E-02, 4.031E-05, 7.149E-05, 1.263E-04,
     5 2.223E-04, 3.879E-04, 6.677E-04, 1.124E-03, 1.847E-03, 2.903E-03,
     6 4.337E-03, 6.138E-03, 8.283E-03, 1.064E-02, 1.312E-02, 1.566E-02,
     7 1.820E-02, 2.075E-02, 2.318E-02, 2.552E-02, 2.776E-02, 2.989E-02,
     8 3.192E-02, 3.384E-02, 3.567E-02, 3.739E-02, 3.950E-04, 6.918E-04,
     9 1.189E-03, 1.996E-03, 3.264E-03, 5.096E-03, 7.557E-03, 1.060E-02/
      COMMON/EST/ZB 3(54)
      DATA ZB 3/
     1 1.416E-02, 1.801E-02, 2.200E-02, 2.601E-02, 2.995E-02, 3.382E-02,
     2 3.747E-02, 4.093E-02, 4.419E-02, 4.725E-02, 5.013E-02, 5.283E-02,
     3 5.535E-02, 5.772E-02, 5.994E-02, 6.203E-02, 6.399E-02, 2.214E-03,
     4 3.697E-03, 5.987E-03, 9.230E-03, 1.348E-02, 1.861E-02, 2.446E-02,
     5 3.061E-02, 3.685E-02, 4.298E-02, 4.887E-02, 5.446E-02, 5.981E-02,
     6 6.471E-02, 6.927E-02, 7.349E-02, 7.741E-02, 8.103E-02, 8.439E-02,
     7 8.751E-02, 9.041E-02, 9.310E-02, 9.561E-02, 9.795E-02, 1.001E-01,
     8 7.936E-03, 1.251E-02, 1.867E-02, 2.629E-02, 3.501E-02, 4.446E-02,
     9 5.399E-02, 6.331E-02, 7.220E-02, 8.052E-02, 8.823E-02, 9.533E-02/
      COMMON/EST/ZB 4(54)
      DATA ZB 4/
     1 1.018E-01, 1.079E-01, 1.134E-01, 1.184E-01, 1.230E-01, 1.272E-01,
     2 1.311E-01, 1.346E-01, 1.379E-01, 1.410E-01, 1.438E-01, 1.464E-01,
     3 1.489E-01, 2.062E-02, 3.056E-02, 4.261E-02, 5.613E-02, 7.047E-02,
     4 8.465E-02, 9.826E-02, 1.110E-01, 1.227E-01, 1.334E-01, 1.431E-01,
     5 1.518E-01, 1.597E-01, 1.668E-01, 1.733E-01, 1.792E-01, 1.845E-01,
     6 1.894E-01, 1.938E-01, 1.979E-01, 2.016E-01, 2.051E-01, 2.083E-01,
     7 2.112E-01, 2.140E-01, 4.294E-02, 6.053E-02, 8.040E-02, 1.013E-01,
     8 1.223E-01, 1.421E-01, 1.605E-01, 1.772E-01, 1.922E-01, 2.057E-01,
     9 2.177E-01, 2.284E-01, 2.380E-01, 2.465E-01, 2.542E-01, 2.612E-01/
      COMMON/EST/ZB 5(54)
      DATA ZB 5/
     1 2.674E-01, 2.731E-01, 2.783E-01, 2.830E-01, 2.873E-01, 2.913E-01,
     2 2.950E-01, 2.983E-01, 3.015E-01, 7.700E-02, 1.047E-01, 1.346E-01,
     3 1.647E-01, 1.936E-01, 2.207E-01, 2.450E-01, 2.667E-01, 2.859E-01,
     4 3.029E-01, 3.178E-01, 3.310E-01, 3.426E-01, 3.530E-01, 3.624E-01,
     5 3.708E-01, 3.782E-01, 3.850E-01, 3.911E-01, 3.966E-01, 4.016E-01,
     6 4.061E-01, 4.103E-01, 4.146E-01, 4.182E-01, 1.244E-01, 1.652E-01,
     7 2.078E-01, 2.497E-01, 2.891E-01, 3.250E-01, 3.570E-01, 3.850E-01,
```

```
     8 4.100E-01, 4.316E-01, 4.505E-01, 4.671E-01, 4.817E-01, 4.948E-01,
     9 5.054E-01, 5.145E-01, 5.226E-01, 5.299E-01, 5.368E-01, 5.427E-01/
       COMMON/EST/ZB 6(54)
       DATA ZB 6/
     1 5.481E-01, 5.530E-01, 5.575E-01, 5.616E-01, 5.654E-01, 1.863E-01,
     2 2.434E-01, 3.020E-01, 3.588E-01, 4.117E-01, 4.595E-01, 5.017E-01,
     3 5.385E-01, 5.624E-01, 5.855E-01, 6.052E-01, 6.218E-01, 6.370E-01,
     4 6.499E-01, 6.613E-01, 6.715E-01, 6.806E-01, 6.887E-01, 6.960E-01,
     5 7.026E-01, 7.087E-01, 7.142E-01, 7.192E-01, 7.239E-01, 7.281E-01,
     6 2.629E-01, 3.396E-01, 4.174E-01, 4.923E-01, 5.592E-01, 6.139E-01,
     7 6.593E-01, 6.960E-01, 7.272E-01, 7.534E-01, 7.758E-01, 7.950E-01,
     8 8.117E-01, 8.262E-01, 8.390E-01, 8.504E-01, 8.605E-01, 8.695E-01,
     9 8.777E-01, 8.851E-01, 8.918E-01, 8.979E-01, 9.035E-01, 9.087E-01/
       COMMON/EST/ZB 7(54)
       DATA ZB 7/
     1 9.135E-01, 3.533E-01, 4.511E-01, 5.555E-01, 6.501E-01, 7.268E-01,
     2 7.895E-01, 8.404E-01, 8.818E-01, 9.168E-01, 9.463E-01, 9.714E-01,
     3 9.929E-01, 1.012E 00, 1.028E 00, 1.042E 00, 1.055E 00, 1.066E 00,
     4 1.076E 00, 1.085E 00, 1.093E 00, 1.101E 00, 1.108E 00, 1.114E 00,
     5 1.120E 00, 1.125E 00, 4.540E-01, 5.919E-01, 7.244E-01, 8.329E-01,
     6 9.206E-01, 9.913E-01, 1.049E 00, 1.096E 00, 1.135E 00, 1.168E 00,
     7 1.196E 00, 1.220E 00, 1.241E 00, 1.259E 00, 1.275E 00, 1.289E 00,
     8 1.302E 00, 1.313E 00, 1.323E 00, 1.332E 00, 1.340E 00, 1.348E 00,
     9 1.355E 00, 1.361E 00, 1.367E 00, 6.232E-01, 7.683E-01, 9.209E-01/
       COMMON/EST/ZB 8(47)
       DATA ZB 8/
     1 1.045E 00, 1.144E 00, 1.224E 00, 1.289E 00, 1.341E 00, 1.386E 00,
     2 1.422E 00, 1.453E 00, 1.480E 00, 1.504E 00, 1.525E 00, 1.544E 00,
     3 1.560E 00, 1.575E 00, 1.588E 00, 1.600E 00, 1.611E 00, 1.621E 00,
     4 1.628E 00, 1.636E 00, 1.644E 00, 1.650E 00, 8.692E-01, 9.739E-01,
     5 1.149E 00, 1.290E 00, 1.402E 00, 1.492E 00, 1.569E 00, 1.633E 00,
     6 1.686E 00, 1.730E 00, 1.768E 00, 1.799E 00, 1.827E 00, 1.851E 00,
     7 1.872E 00, 1.890E 00, 1.907E 00, 1.922E 00, 1.935E 00, 1.947E 00,
     8 1.958E 00, 1.968E 00, 1.977E 00, 1.985E 00, 1.993E 00/
       COMMON/EST/ZB 9(29)
       DATA ZB 9/
     5              9.721E-1,  1.216E+0,  1.415E+0,  1.580E+0,  1.718E+0,
     6  1.829E+0,  1.918E+0,  1.991E+0,  2.051E+0,  2.100E+0,  2.143E+0,
     7  2.180E+0,  2.211E+0,  2.239E+0,  2.263E+0,  2.284E+0,  2.303E+0,
     8  2.320E+0,  2.335E+0,  2.348E+0,  2.361E+0,  2.372E+0,  2.382E+0,
     9  2.391E+0,  2.401E+0,  1.217E+0,  1.497E+0,  1.743E+0,  1.944E+0/
       COMMON/EST/ZB10(54)
       DATA ZB10/
     1  2.103E+0,  2.229E+0,  2.331E+0,  2.415E+0,  2.485E+0,  2.538E+0,
     2  2.584E+0,  2.623E+0,  2.656E+0,  2.685E+0,  2.711E+0,  2.733E+0,
     3  2.754E+0,  2.772E+0,  2.788E+0,  2.803E+0,  2.817E+0,  2.828E+0,
     4  2.839E+0,  2.850E+0,  2.859E+0,  1.505E+0,  1.854E+0,  2.143E+0,
     5  2.373E+0,  2.550E+0,  2.681E+0,  2.786E+0,  2.872E+0,  2.943E+0,
     6  3.003E+0,  3.054E+0,  3.097E+0,  3.135E+0,  3.168E+0,  3.197E+0,
     7  3.223E+0,  3.246E+0,  3.266E+0,  3.285E+0,  3.301E+0,  3.317E+0,
     8  3.331E+0,  3.343E+0,  3.355E+0,  3.366E+0,  1.870E+0,  2.278E+0,
     9  2.600E+0,  2.834E+0,  3.019E+0,  3.164E+0,  3.284E+0,  3.381E+0/
       COMMON/EST/ZB11(54)
       DATA ZB11/
     1  3.461E+0,  3.527E+0,  3.582E+0,  3.630E+0,  3.672E+0,  3.708E+0,
     2  3.739E+0,  3.768E+0,  3.793E+0,  3.815E+0,  3.836E+0,  3.854E+0,
     3  3.871E+0,  3.886E+0,  3.900E+0,  3.913E+0,  3.925E+0,  2.303E+0,
     4  2.746E+0,  3.082E+0,  3.344E+0,  3.548E+0,  3.706E+0,  3.834E+0,
     5  3.938E+0,  4.025E+0,  4.098E+0,  4.161E+0,  4.214E+0,  4.261E+0,
     6  4.301E+0,  4.337E+0,  4.369E+0,  4.397E+0,  4.422E+0,  4.445E+0,
     7  4.466E+0,  4.485E+0,  4.502E+0,  4.518E+0,  4.532E+0,  4.545E+0,
     8  2.780E+0,  3.256E+0,  3.627E+0,  3.909E+0,  4.130E+0,  4.307E+0,
     9  4.449E+0,  4.566E+0,  4.661E+0,  4.743E+0,  4.812E+0,  4.872E+0/
       COMMON/EST/ZB12(54)
       DATA ZB12/
```

```
1  4.924E+0,  4.969E+0,  5.009E+0,  5.045E+0,  5.076E+0,  5.105E+0,
2  5.130E+0,  5.153E+0,  5.174E+0,  5.194E+0,  5.211E+0,  5.228E+0,
3  5.243E+0,  3.307E+0,  3.828E+0,  4.230E+0,  4.544E+0,  4.789E+0,
4  4.986E+0,  5.145E+0,  5.274E+0,  5.383E+0,  5.474E+0,  5.536E+0,
5  5.582E+0,  5.623E+0,  5.659E+0,  5.692E+0,  5.721E+0,  5.748E+0,
6  5.772E+0,  5.794E+0,  5.814E+0,  5.833E+0,  5.850E+0,  5.866E+0,
7  5.880E+0,  5.894E+0,  3.901E+0,  4.474E+0,  4.921E+0,  5.267E+0,
8  5.526E+0,  5.658E+0,  5.767E+0,  5.859E+0,  5.939E+0,  6.007E+0,
9  6.067E+0,  6.119E+0,  6.166E+0,  6.207E+0,  6.244E+0,  6.277E+0/
  COMMON/EST/ZB13( 9)
  DATA ZB13/
1  6.306E+0,  6.334E+0,  6.358E+0,  6.381E+0,  6.402E+0,  6.419E+0,
2  6.437E+0,  6.453E+0,  6.468E+0/
  COMMON/EST/EILN 1(54)
  DATA EILN 1/
1-1.961E 01,-1.961E 01,-1.961E 01,-1.822E 01,-1.782E 01,-1.731E 01,
2-1.672E 01,-1.614E 01,-1.555E 01,-1.498E 01,-1.440E 01,-1.383E 01,
3-1.325E 01,-1.268E 01,-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,
4-9.802E 00,-9.229E 00,-8.659E 00,-8.093E 00,-7.534E 00,-6.987E 00,
5-6.461E 00,-1.499E 01,-1.440E 01,-1.383E 01,-1.325E 01,-1.268E 01,
6-1.210E 01,-1.153E 01,-1.095E 01,-1.038E 01,-9.800E 00,-9.227E 00,
7-8.654E 00,-8.084E 00,-7.518E 00,-6.959E 00,-6.413E 00,-5.887E 00,
8-5.393E 00,-4.921E 00,-4.507E 00,-4.145E 00,-3.829E 00,-3.562E 00,
9-3.336E 00,-3.144E 00,-1.104E 01,-1.047E 01,-9.892E 00,-9.317E 00/
  COMMON/EST/EILN 2(54)
  DATA EILN 2/
1-8.743E 00,-8.171E 00,-7.600E 00,-7.034E 00,-6.474E 00,-5.926E 00,
2-5.398E 00,-4.899E 00,-4.425E 00,-4.006E 00,-3.641E 00 -3.329E 00,
3-3.055E 00,-2.829E 00,-2.638E 00,-2.475E 00,-2.331E 00,-2.209E 00,
4-2.103E 00,-2.009E 00,-1.927E 00,-8.041E 00,-7.468E 00,-6.899E 00,
5-6.334E 00,-5.777E 00,-5.234E 00,-4.713E 00,-4.216E 00,-3.764E 00,
6-3.363E 00,-3.016E 00,-2.716E 00,-2.466E 00,-2.256E 00,-2.079E 00,
7-1.929E 00,-1.797E 00,-1.687E 00,-1.591E 00,-1.506E 00,-1.432E 00,
8-1.367E 00,-1.308E 00,-1.256E 00,-1.209E 00,-5.759E 00,-5.199E 00,
9-4.657E 00,-4.139E 00,-3.647E 00,-3.202E 00,-2.808E 00,-2.469E 00/
  COMMON/EST/EILN 3(54)
  DATA EILN 3/
1-2.179E 00,-1.939E 00,-1.739E 00,-1.572E 00,-1.431E 00,-1.309E 00,
2-1.207E 00,-1.118E 00,-1.042E 00,-9.745E-01,-9.154E-01,-8.630E-01,
3-8.163E-01,-7.744E-01,-7.366E-01,-7.024E-01,-6.714E-01,-4.035E 00,
4-3.523E 00,-3.040E 00,-2.608E 00,-2.229E 00,-1.906E 00,-1.633E 00,
5-1.409E 00,-1.223E 00,-1.069E 00,-9.409E-01,-8.327E-01,-7.390E-01,
6-6.601E-01,-5.921E-01,-5.329E-01,-4.810E-01,-4.352E-01,-3.946E-01,
7-3.583E-01,-3.257E-01,-2.964E-01,-2.698E-01,-2.456E-01,-2.235E-01,
8-2.759E 00,-2.303E 00,-1.903E 00,-1.561E 00,-1.275E 00,-1.035E 00,
9-8.412E-01,-6.819E-01,-5.506E-01,-4.415E-01,-3.501E-01,-2.727E-01/
  COMMON/EST/EILN 4(54)
  DATA EILN 4/
1-2.067E-01,-1.484E-01,-9.905E-02,-5.591E-02,-1.794E-02, 1.568E-02,
2 4.563E-02, 7.246E-02, 9.660E-02, 1.184E-01, 1.383E-01, 1.564E-01,
3 1.729E-01,-1.804E 00,-1.411E 00,-1.078E 00,-8.024E-01,-5.749E-01,
4-3.915E-01,-2.424E-01,-1.206E-01,-2.026E-02, 6.316E-02, 1.332E-01,
5 1.925E-01, 2.432E-01, 2.870E-01, 3.250E-01, 3.583E-01, 3.876E-01,
6 4.136E-01, 4.368E-01, 4.576E-01, 4.764E-01, 4.934E-01, 5.088E-01,
7 5.229E-01, 5.358E-01,-1.070E 00,-7.269E-01,-4.430E-01,-2.121E-01,
8-2.386E-02, 1.265E-01, 2.481E-01, 3.471E-01, 4.286E-01, 4.962E-01,
9 5.529E-01, 6.010E-01, 6.420E-01, 6.774E-01, 7.082E-01, 7.351E-01/
  COMMON/EST/EILN 5(54)
  DATA EILN 5/
1 7.588E-01, 7.799E-01, 7.986E-01, 8.154E-01, 8.306E-01, 8.443E-01,
2 8.568E-01, 8.682E-01, 8.786E-01,-4.863E-01,-1.788E-01, 7.220E-02,
3 2.742E-01, 4.359E-01, 5.668E-01, 6.712E-01, 7.560E-01, 8.256E-01,
4 8.832E-01, 9.314E-01, 9.722E-01, 1.006E 00, 1.037E 00, 1.063E 00,
5 1.086E 00, 1.105E 00, 1.123E 00, 1.139E 00, 1.153E 00, 1.165E 00,
6 1.177E 00, 1.187E 00, 1.197E 00, 1.206E 00,-6.935E-03, 2.768E-01,
```

```
     7 5.063E-01, 6.901E-01, 8.367E-01, 9.538E-01, 1.048E 00, 1.123E 00,
     8 1.186E 00, 1.238E 00, 1.280E 00, 1.317E 00, 1.347E 00, 1.374E 00,
     9 1.395E 00, 1.413E 00, 1.429E 00, 1.444E 00, 1.457E 00, 1.469E 00/
       COMMON/EST/EILN 6(54)
       DATA EILN 6/
     1 1.479E 00, 1.488E 00, 1.497E 00, 1.505E 00, 1.512E 00, 3.972E-01,
     2 6.645E-01, 8.802E-01, 1.053E 00, 1.190E 00, 1.300E 00, 1.388E 00,
     3 1.453E 00, 1.506E 00, 1.550E 00, 1.587E 00, 1.617E 00, 1.644E 00,
     4 1.668E 00, 1.688E 00, 1.706E 00, 1.722E 00, 1.736E 00, 1.748E 00,
     5 1.760E 00, 1.770E 00, 1.779E 00, 1.788E 00, 1.796E 00, 1.803E 00,
     6 7.419E-01, 9.970E-01, 1.204E 00, 1.369E 00, 1.500E 00, 1.603E 00,
     7 1.684E 00, 1.748E 00, 1.801E 00, 1.845E 00, 1.882E 00, 1.913E 00,
     8 1.939E 00, 1.962E 00, 1.982E 00, 2.000E 00, 2.015E 00, 2.029E 00,
     9 2.042E 00, 2.053E 00, 2.063E 00, 2.072E 00, 2.080E 00, 2.088E 00/
       COMMON/EST/EILN 7(54)
       DATA EILN 7/
     1 2.095E 00, 1.037E 00, 1.282E 00, 1.493E 00, 1.668E 00, 1.801E 00,
     2 1.904E 00, 1.985E 00, 2.048E 00, 2.100E 00, 2.143E 00, 2.179E 00,
     3 2.209E 00, 2.235E 00, 2.258E 00, 2.277E 00, 2.295E 00, 2.310E 00,
     4 2.323E 00, 2.335E 00, 2.346E 00, 2.356E 00, 2.365E 00, 2.373E 00,
     5 2.381E 00, 2.387E 00, 1.288E 00, 1.562E 00, 1.797E 00, 1.973E 00,
     6 2.106E 00, 2.207E 00, 2.286E 00, 2.349E 00, 2.400E 00, 2.442E 00,
     7 2.477E 00, 2.506E 00, 2.532E 00, 2.554E 00, 2.573E 00, 2.589E 00,
     8 2.604E 00, 2.617E 00, 2.629E 00, 2.640E 00, 2.649E 00, 2.658E 00,
     9 2.666E 00, 2.673E 00, 2.680E 00, 1.619E 00, 1.870E 00, 2.106E 00/
       COMMON/EST/EILN 8(47)
       DATA EILN 8/
     1 2.281E 00, 2.412E 00, 2.512E 00, 2.589E 00, 2.650E 00, 2.700E 00,
     2 2.741E 00, 2.774E 00, 2.803E 00, 2.828E 00, 2.850E 00, 2.869E 00,
     3 2.886E 00, 2.901E 00, 2.914E 00, 2.926E 00, 2.936E 00, 2.944E 00,
     4 2.953E 00, 2.961E 00, 2.968E 00, 2.974E 00, 2.029E 00, 2.183E 00,
     5 2.419E 00, 2.591E 00, 2.718E 00, 2.815E 00, 2.895E 00, 2.958E 00,
     6 3.008E 00, 3.049E 00, 3.082E 00, 3.110E 00, 3.134E 00, 3.154E 00,
     7 3.172E 00, 3.188E 00, 3.202E 00, 3.214E 00, 3.225E 00, 3.234E 00,
     8 3.243E 00, 3.251E 00, 3.258E 00, 3.265E 00, 3.271E 00/
       COMMON/EST/EILN 9(29)
       DATA EILN 9/
     5           2.180E+0,  2.501E+0,  2.732E+0,  2.906E+0,  3.038E+0,
     6  3.136E+0,  3.211E+0,  3.270E+0,  3.318E+0,  3.354E+0,  3.386E+0,
     7  3.412E+0,  3.435E+0,  3.455E+0,  3.472E+0,  3.487E+0,  3.500E+0,
     8  3.511E+0,  3.522E+0,  3.530E+0,  3.539E+0,  3.546E+0,  3.553E+0,
     9  3.559E+0,  3.565E+0,  2.504E+0,  2.820E+0,  3.061E+0,  3.232E+0/
       COMMON/EST/EILN10(54)
       DATA EILN10/
     1  3.356E+0,  3.447E+0,  3.519E+0,  3.575E+0,  3.620E+0,  3.654E+0,
     2  3.683E+0,  3.707E+0,  3.728E+0,  3.746E+0,  3.762E+0,  3.775E+0,
     3  3.788E+0,  3.799E+0,  3.808E+0,  3.817E+0,  3.826E+0,  3.833E+0,
     4  3.839E+0,  3.846E+0,  3.851E+0,  2.829E+0,  3.157E+0,  3.385E+0,
     5  3.547E+0,  3.662E+0,  3.744E+0,  3.807E+0,  3.858E+0,  3.900E+0,
     6  3.935E+0,  3.965E+0,  3.989E+0,  4.011E+0,  4.029E+0,  4.045E+0,
     7  4.060E+0,  4.072E+0,  4.083E+0,  4.093E+0,  4.103E+0,  4.111E+0,
     8  4.118E+0,  4.125E+0,  4.131E+0,  4.137E+0,  3.171E+0,  3.482E+0,
     9  3.693E+0,  3.836E+0,  3.945E+0,  4.027E+0,  4.093E+0,  4.145E+0/
       COMMON/EST/EILN11(54)
       DATA EILN11/
     1  4.188E+0,  4.222E+0,  4.251E+0,  4.275E+0,  4.296E+0,  4.315E+0,
     2  4.331E+0,  4.345E+0,  4.357E+0,  4.369E+0,  4.379E+0,  4.388E+0,
     3  4.396E+0,  4.403E+0,  4.410E+0,  4.417E+0,  4.422E+0,  3.500E+0,
     4  3.783E+0,  3.980E+0,  4.125E+0,  4.233E+0,  4.314E+0,  4.378E+0,
     5  4.429E+0,  4.471E+0,  4.506E+0,  4.535E+0,  4.560E+0,  4.581E+0,
     6  4.600E+0,  4.616E+0,  4.630E+0,  4.643E+0,  4.655E+0,  4.665E+0,
     7  4.674E+0,  4.682E+0,  4.690E+0,  4.697E+0,  4.703E+0,  4.709E+0,
     8  3.804E+0,  4.078E+0,  4.274E+0,  4.415E+0,  4.521E+0,  4.602E+0,
     9  4.667E+0,  4.718E+0,  4.759E+0,  4.794E+0,  4.823E+0,  4.848E+0/
       COMMON/EST/EILN12(54)
```

```
      DATA EILN12/
     1  4.870E+0,  4.888E+0,  4.905E+0,  4.919E+0,  4.932E+0,  4.943E+0,
     2  4.953E+0,  4.962E+0,  4.971E+0,  4.978E+0,  4.985E+0,  4.992E+0,
     3  4.997E+0,  4.105E+0,  4.375E+0,  4.567E+0,  4.709E+0,  4.814E+0,
     4  4.895E+0,  4.959E+0,  5.010E+0,  5.052E+0,  5.086E+0,  5.109E+0,
     5  5.127E+0,  5.143E+0,  5.158E+0,  5.171E+0,  5.183E+0,  5.194E+0,
     6  5.204E+0,  5.214E+0,  5.222E+0,  5.230E+0,  5.238E+0,  5.245E+0,
     7  5.251E+0,  5.257E+0,  4.411E+0,  4.678E+0,  4.869E+0,  5.007E+0,
     8  5.105E+0,  5.157E+0,  5.202E+0,  5.242E+0,  5.277E+0,  5.308E+0,
     9  5.335E+0,  5.359E+0,  5.380E+0,  5.399E+0,  5.416E+0,  5.432E+0/
      COMMON/EST/EILN13( 9)
      DATA EILN13/
     1  5.446E+0,  5.458E+0,  5.470E+0,  5.481E+0,  5.490E+0,  5.499E+0,
     2  5.507E+0,  5.515E+0,  5.522E+0/
      IF(E.NE.0.) GO TO 5
      THA = 1.E-3
      ZBAR=0.
      GO TO 950
    5 CONTINUE
      ALGT=ALOG10(TAU)
      ALGE=ALOG10(E)
      DLGT=ALGT-TAULZ
      DLGE=ALGE-ELZ
      AN=DLGT*S+1.
      AM=DLGE*T+1.
      IF (DLGT.LT.0.) AN=0.
      IF(DLGE.LT.0.) AM=0.
      N=IFIX(AN)
      M=IFIX(AM)
      IN=0
      EO=E
      IF(N.LE.0) GO TO 10
      IF(N.GE.NN) GO TO 20
      IF(M.LE.0) GO TO 800
      IF(M.GE.MM) GO TO 400
    8 CONTINUE
      DNLT=AN-AINT(AN)
      DMLE=AM-AINT(AM)
      ZBAR=ZB(N,M)+(ZB(N+1,M)-ZB(N,M))* DNLT
     1             +(ZB(N,M+1)-ZB(N,M))* DMLE
     2             +(ZB(N+1,M+1)+ZB(N,M)-ZB(N+1,M)-ZB(N,M+1))
     3             *(DNLT*DMLE)
      ALIN=EILN(N,M)+(EILN(N+1,M)-EILN(N,M))*DNLT
     1             +(EILN(N,M+1)-EILN(N,M))*DMLE
     3             *(DNLT*DMLE)
     2             +(EILN(N+1,M+1)+EILN(N,M)-EILN(N+1,M)-EILN(N,M+1))
      THA=(EO/PHI-EXP(ALIN))/(1.5*(1.+ZBAR   ))
      IF(IN.NE.0)GO TO (150,250,350,450,550,650,750,850),IN
      GO TO 950
   10 IF(M.LE.0) GO TO 100
      IF(M.GE.MM) GO TO 300
      GO TO 200
   20 IF(M.LE.0) GO TO 700
      IF(M.GE.MM) GO TO 500
      GO TO 600
  100 CONTINUE
      IF(I1.EQ.1) GO TO 9901
  150 CONTINUE
      RETURN
  200 CONTINUE
      IF(I2.EQ.1) GO TO 9902
  250 CONTINUE
      RETURN
  300 CONTINUE
      IF(I3.EQ.1) GO TO 9903
```

```
  350 CONTINUE
      RETURN
  400 CONTINUE
      IF(I4.EQ.1) GO TO 9904
  450 CONTINUE
      RETURN
  500 CONTINUE
      IF(I5.EQ.1) GO TO 9905
  550 CONTINUE
      RETURN
  600 CONTINUE
      IF(I6.EQ.1) GO TO 9906
  650 CONTINUE
      RETURN
  700 CONTINUE
      IF(I7.EQ.1) GO TO 9907
      IN = 7
      M = 1
      N = NN
      EO=EZ
      GO TO 8
  750 THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * SQRT(TAUM/TAU)*EXP(V1*(THAP-THA) /
     1 (THA*THAP*2.))
      AIN=V1*ZBAR
      GO TO 900
  800 CONTINUE
      IF(I8.EQ.1) GO TO 9908
      IN = 8
      M = 1
      EO=EZ
      GO TO 8
  850 THAP = E * THA / EZ
      ZBAR = ZBAR * (THAP/THA)**.75 * EXP(V1*( THAP - THA) /
     1(THA * THAP*2.))
      AIN=V1*ZBAR
  900 CONTINUE
      THA=(E/PHI-AIN)/(1.5*(1.+ZBAR))
  950 P=PHI*(1.+ZBAR    )*THA/TAU
      RETURN
 9901 S1=12.0100
      GO TO 9999
 9902 S1=12.0200
      GO TO 9999
 9903 S1=12.0300
      GO TO 9999
 9904 S1=12.0400
      GO TO 9999
 9905 S1=12.0500
      GO TO 9999
 9906 S1=12.0600
      GO TO 9999
 9907 S1=12.0700
      GO TO 9999
 9908 S1=12.0800
 9999 WRITE(6,1000)TAU,E,THA,P,ZBAR,GG,ALGT
 1000 FORMAT(1H1,12X,6HTAU    ,9X,6HE      ,9X,6HTHA    ,9X,6HP      ,9X,6HZ
     1BAR   ,9X,6HGG     ,9X,6HALGT   /7X,1P7E15.7)
      WRITE(6,1001)ALGE,DLGT,DLGE,AN,AM
 1001 FORMAT(1H0,12X,6HALGE   ,9X,6HDLGT   ,9X,6HDLGE   ,9X,6HAN     ,9X,6HA
     1M     /7X,1P5E15.7)
      WRITE(6,1002)N,M,NN,MM,S1
 1002 FORMAT(1H0,12X,6HN      ,9X,6HM      ,9X,6HNN     ,9X,6HMM     ,9X,6HS
     11     /7X,I9,3(6X,I9),1PE15.7)
      CALL EDIT
      END
```

SECTION V

EQUATION OF STATE FOR MOLECULAR CARBON

5. 1. INTRODUCTION

In the theoretical analysis of certain experimental systems, it is convenient to treat the vapor phase of a graphite-carbon vapor system as though it were in local thermodynamic equilibrium. It is then possible to calculate the equilibrium composition of the vapor. In this section a FORTRAN subroutine, CMOL, is described which, given the local temperature and specific volume, will calculate the composition and thermodynamic properties of molecular carbon vapor.

Two gross assumptions must first be stated: (1) it is assumed that only the species $C_1, C_2, \ldots, C_{10}$ are present, and (2) the perfect gas law is assumed at several places. In addition to these assumptions, an extrapolation past the known data to the limiting high-temperature values of monatomic carbon vapor permits the user to bridge, in a physically consistent manner, the region where the free energies of the system have not yet been determined.

Finally, the systems of interest are metastable in that the carbon vapor formed is not expected to condense to graphite within the time period under study. Thus, the routine permits the calculation of the system composition under the assumption that only vapor is present.

5. 2. SYMBOLS

$A_{\alpha,j}$ j^{th} coefficient in the least-square fit to the enthalpy and free energy of species α,

a_α A^{th} coefficient in $f(\xi_1)$; see Eq. (122e)

C_j Molecule in carbon vapor containing j atoms of carbon,

E_{sp} Specific internal energy in calories/gram,

E_α Internal energy per mole of species α in calories/mole,

$f(\xi_1)$ See Eq. (122e),

$G^o_\alpha(0)$ Gibbs free energy of species α at O°K,

$G^o_\alpha(T)$ Gibbs free energy of species α at T°K,

G_α $G_\alpha \equiv G^o_\alpha(T)$,

ΔG^o_α Change in free energy due to reaction, for the reaction $\alpha C_1 \rightleftharpoons C_\alpha$: $\Delta G^o_\alpha = G_\alpha - \alpha G_1$,

$H^o_\alpha(0)$ Enthalpy of species α at O°K,

$H^o_\alpha(T)$ Enthalpy of species α at T°K,

H_α $H_\alpha \equiv H^o_\alpha(T)$,

K^α_c Equilibrium constant, i. t. o. concentrations, for the reaction $\alpha C_1 \rightleftharpoons C_\alpha$: $K^\alpha_c = (RT)^{\alpha-1} K^\alpha_p$; $K^\alpha_c = K^\alpha_c(T, \xi_\alpha)$,

K^α_p Equilibrium constant i. t. o. partial pressures, for the reaction $\alpha C_1 \rightleftharpoons C_\alpha$: $K^\alpha_p = \exp(-\Delta G^o_\alpha/RT)$; $K^\alpha_p = K^\alpha_p(T)$,

M Mass of the system; $M = \Sigma_\alpha M_\alpha = \Sigma_\alpha n_\alpha M^o_\alpha$ in grams,

M^o_α Gram-molecular weight of species α in grams/mole,

$\bar{N}$ Mean number of atoms/molecule; see Eq. (140a),

n_α Number of moles of species α,

n $n = \Sigma_\alpha n_\alpha$, the total number of moles,

P $P = \Sigma_\alpha P_\alpha = RT \Sigma_\alpha \xi_\alpha$; system pressure in dynes/cm^2,

P_α Pressure of component α,

R	Gas constant. The units of R are consistent with the other factors in the equation in which it appears; for example, in Eqs. (120), (132), etc., R = 1.9876 calorie/mole-°K; in Eqs. (114), etc., R = 8.3143×10^7 erg/mole-°K,
T	Temperature in °K,
V	Total system volume in cm^3,
α	Molecular species index: $1 \leq \alpha \leq 10$,
ρ	Mass density in g/cm^3; $\rho = M/V = 1/\tau$,
τ	Specific volume in cm/g; $\tau = V/M = 1/\rho$,
θ	Temperature in ev,
ξ_α	$\xi_\alpha = n_\alpha V$, the number density in moles/cm^3 of species α.

5.3. THE SYSTEM COMPOSITION

The equilibria assumed can be written as

$$\alpha\, C_1 \rightleftharpoons C_\alpha \; ; \qquad \alpha = 2, 3, \ldots, 10 \tag{112}$$

and they lead to

$$\frac{P_\alpha}{(P_1)^\alpha} = K_p^\alpha(T) \tag{113}$$

Or, assuming that

$$P_\alpha V = n_\alpha RT$$

$$P_\alpha = \frac{n_\alpha}{V} RT = \xi_\alpha RT \tag{114}$$

where $\xi_\alpha = n_\alpha/V$, we obtain

$$\xi_\alpha = (RT)^{\alpha-1} (\xi_1)^\alpha K_p^\alpha(T)$$

$$= \left[K_c^\alpha(T, \xi_\alpha)\right] \left[\xi_1\right]^\alpha \tag{115}$$

where

$$K_p^{\alpha} = \exp(-\Delta G_{\alpha}/RT)$$
$$= \exp\left(\left[\alpha\ G_1 - G_{\alpha}\right]/RT\right) \tag{116}$$

and G_{α} is the Gibbs free energy of species α:

$$\frac{G_{\alpha}}{RT} \equiv \frac{G_{\alpha}^{o}(T)}{RT} \tag{117}$$

These free energy functions, and others, appear in a paper by Duff and Bauer (Ref. 1)* in the form of a least-square fit to the data over two overlapping ranges and are written as

$$\frac{G_{\alpha}^{o}(T)}{RT} = A_{\alpha,1}(1 - \ln T) - \left(\Sigma_{j=2}^{j=4}\left[A_{\alpha,j}\,T^{j}\right]/j\right) - A_{\alpha,5} + H_{\alpha}^{o}(0)/RT \tag{118}$$

This fit simultaneously gives the enthalpy of species α as

$$\frac{H_{\alpha}}{RT} \equiv \frac{H_{\alpha}^{o}(T)}{RT} = \left(\Sigma_{j=1}^{j=4} A_{\alpha,j}\,T^{j-1}\right) + H_{\alpha}^{o}(0)/RT \tag{119}$$

and thus satisfies the thermodynamic consistency relation:

$$-T\left(\frac{d(G_{\alpha}/RT)}{dT}\right) = (H_{\alpha}/RT) \tag{120}$$

We thus have 9 equations in the 10 species. The final equation needed is given by the mass conservation relation:

$$M = \Sigma_{\alpha} n_{\alpha} M_{\alpha}^{o} \tag{121}$$

---

* It should be noted that the thermodynamic function table titles are inverted in this reference; i.e., the table titled "from 300° K-1500° K" actually is the table for 1500° K-6000° K, and vice versa.

which transforms to

$$\rho = \frac{M}{V} = \Sigma_\alpha \frac{n_\alpha}{V} M_\alpha^o \qquad (122a)$$

$$= \Sigma_\alpha \xi_\alpha M_\alpha^o \qquad (122b)$$

$$= \Sigma_\alpha \xi_\alpha (12\alpha) \qquad (122c)$$

or

$$0 = \sum_{\alpha=1}^{10} \alpha e^{-\Delta G_\alpha/RT} (RT)^{\alpha-1} (\xi_1)^\alpha - \rho/12 \qquad (122d)$$

which we immediately recognize as a tenth-order polynomial in ξ_1, the number density, in moles/cm^3, of carbon atoms. For convenience we assume the standard polynomial form:

$$0 = f(\xi_1) = \Sigma_{\alpha=0}^{\alpha=10} a_\alpha (\xi_1)^\alpha \qquad (122e)$$

We note that, by definition of the variables ξ_α,

$$0 < \xi_1 < \rho/12 \qquad (123a)$$

For these limiting values of the argument, the polynomial assumes the values

$$f(0) = -\rho/12 \qquad (123b)$$

and

$$f(\rho/12) > 0 \ . \qquad (123c)$$

Further, Descartes' rule of signs permits, at most, one real root. Since there is at least one real root, this root must be unique. We thus have all the information needed to find the root.

Because of limitations imposed by the permissible exponent range inherent in most computer systems, Eq. (122e) was rewritten as

$$0 = \Sigma_{\alpha=0}^{\alpha=10} a'_\alpha X^\alpha \qquad (124a)$$

where

$$X = \left[\xi_1 \, e^{G_1/RT} \, RT \right] = \frac{\xi_1}{a_1'} \tag{124b}$$

$$a_\alpha' = \alpha \, e^{-G_\alpha/RT} \, /RT \; ; \quad 1 \le \alpha \le 10 \tag{124c}$$

$$a_0' = -\rho/12 = a_0 \tag{124d}$$

The bounds on X are stated immediately in terms of those previously stated for ξ_1 in Eq. (123a):

$$0 < X < -a_0/a_1' \tag{124e}$$

A series of numerical experiments was performed to establish the most efficient manner of solving for this root. The techniques considered were:

(a) Interval halving,

(b) regula falsi (the n^{th} iterate is the inverse linear interpolate between iterates n-1 and n-2),

(c) Newton-Raphson,

(d) The analogue of Newton-Raphson which uses the first and second derivatives.

Numerical experiments showed that the expected gain in the rate of convergence with the higher order methods (c and d) did not occur over much of the (T, ρ) domain of interest. This would clearly not be true if an initial estimate sufficiently close to the final iterate could be found. However, the estimates which were used were not always within this desirable domain:

1. If $Z_1 \equiv (-a'_{10})/a'_1 \leq 1$, $X < Z_1$.

2. If $Z_1 > 1$, and $a'_j \neq 0$ where $j = 9, 8, 7, \ldots, 1$ (and $a_j \neq 0$ for $j = 9, 8, 7, \ldots, 2$), $Z_2 \equiv 1 + \left[-a'_o/a'_j\right]^{1/j}$ and $X < Z_2$.

3. If $Z_2 < 2$, $Z_3 \equiv Z_2 - 1$ and $X < Z_3$

Thus, techniques (c) and (d) were often useless.

For a tenth order polynomial with the constant term as the only negative coefficient, an upper bound on the root is

$$X < 1 + \left[|a'_0|/a'_{10}\right]^{1/10}$$

However, numerical experiments have shown that the bound Z_2 given above is better; this is easily understood when one examines the behavior of the functions $\left|(G_\alpha/RT)\right| 1 \leq \alpha \leq 10\Big|$, for ξ_9 always dominates ξ_{10}.

Technique (c) requires almost twice as much computation as techniques (a) and (b), and technique (d) requires almost three times as much computation. Thus, if second or third order convergence is not rapidly achieved, one is much better off with the lower order methods. For this reason, a careful study of the best way to use techniques (a) and (b) was performed.

Regula falsi and interval halving both require computation of $f(X^{(n)})$ where $X^{(n)}$ is the n^{th} iterate. In addition, interval halving requires comparison of $f(X^{(n)})$ with the upper and lower bounds determined at the $(n-1)^{st}$ iteration stage. If $f(X^{(n)}) > 0$, $X^{(n)}$ replaces the previous upper bound. If $f(X^{(n)}) < 0$, $X^{(n)}$ replaces the previous lower bound. If $|f(X^{(n)})| < \epsilon$, we are sufficiently close to the desired answer and can use $X^{(n)}$ as our final iterate. This process is clearly convergent; approximately

three iterations are required to reduce the error by a factor of 10. Regula falsi will permit a much faster asymptotic convergence rate; however, the initial rate of convergence may be much slower. Therefore, interval halving is used until the criterion

$$\left| \sum_{\alpha-1}^{\alpha=10} a'_\alpha \left[X^{(k)}\right]^\alpha \right| < +0.1\,(\rho/12) \tag{125}$$

is met; from this iteration stage on, regula falsi is used until $|f(X^{(n)})| < \delta$. However, if regula falsi predicts a new iterate outside the current upper and lower bounds, interval halving is used at that iteration stage. The upper and lower bounds are updated at every iteration stage. Twenty-five iterations are allowed; if the accuracy test is not satisfied, the cell CARBNZ (8) is set to 97.0297 and a return is made to the calling program.

When X has been determined to the desired accuracy, the ξ_α, $\alpha = 1, \ldots, 10$ are computed using Eqs. (115) and (116).

5.4. THERMODYNAMIC VARIABLES

The thermodynamic variables computed are:

$$P = RT\ \Sigma_\alpha \xi_\alpha \tag{126}$$

$$\left(\frac{\partial P}{\partial T}\right)_\tau = RT \Sigma_\alpha \left(\frac{d\xi_\alpha}{dT}\right)_\tau + \frac{P}{T} \tag{127}$$

$$\left(\frac{dP}{\partial \tau}\right)_T = RT\ \Sigma_\alpha \left(\frac{\partial \xi_\alpha}{d\tau}\right)_T \tag{128}$$

$$E_{sp} = \tau \Sigma_\alpha\ E_\alpha \xi_\alpha = \Sigma_\alpha\ E_\alpha \xi_\alpha / \left(12\bar{N}\ \Sigma_\alpha \xi_\alpha\right) \tag{129}$$

$$\left(\frac{\partial E_{sp}}{\partial \tau}\right)_T = \tau \left\{ \Sigma_\alpha\ E_\alpha \left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T - 12\, E_{sp} \left[\Sigma_\alpha \left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T \right] \right\} \tag{130}$$

$$\left(\frac{\partial E_{sp}}{\partial T}\right)_\tau = \tau \left\{ \Sigma_\alpha \left[E_\alpha \left(\frac{\partial \xi_\alpha}{\partial \tau}\right) + \left(\frac{dE_\alpha}{dT}\right) \xi_\alpha \right] - 12\, E_{sp} \left[\Sigma_\alpha \alpha \left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau \right] \right\} \tag{131}$$

$$E_\alpha = RT\left[\frac{H_\alpha}{RT} - 1\right] \tag{132}$$

$$\frac{dE_\alpha}{dT} = R\left[\frac{H_\alpha}{RT} - 1\right] + RT\left(\frac{dH_\alpha/RT}{dT}\right) \tag{133}$$

where

$$RT\left(\frac{dH_\alpha/RT}{dT}\right) = R\left[\Sigma_{j=2}^{j=4} (j-1)\, A_{\alpha,j}\, T^{j-1}\right] - \frac{H_\alpha^\circ(0)}{RT} \tag{134}$$

so

$$\frac{dE_\alpha}{dT} = R\left[\Sigma_{j=1}^{j=4} (j)\, A_{\alpha,j}\, T^{(j-1)} - 1\right] \tag{135}$$

$$\left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau = \xi_\alpha \left\{ \alpha\, (\xi_1)^{-1} \left(\frac{d\xi_1}{dT}\right)_\tau + T^{-1} \left[\alpha \left(T\, \frac{dG/RT}{dT} \right) - \left(T\, \frac{dG_\alpha/RT}{dT} \right) + (\alpha - 1) \right] \right\} \tag{136}$$

$$\left(\frac{\partial \xi_\alpha}{d\tau}\right)_T = \alpha \left(\frac{\partial \xi_1}{dT}\right)_\tau \frac{\xi_\alpha}{\xi_1} \tag{137}$$

$$\left(\frac{\partial \xi_1}{\partial T}\right)_\tau = \xi_1\, T^{-1} \left\{ \left[(\rho/12) - \left(\Sigma_\alpha\, \alpha\, \xi_\alpha \left[\alpha \left(T\, \frac{dG_1/RT}{dT} \right) - \left(T\, \frac{dG_\alpha/RT}{dT} \right) \right] \right) / \Sigma_\alpha\, \alpha^2\, \xi_\alpha \right] - 1 \right\} \tag{138}$$

$$\left(\frac{\partial \xi_1}{\partial \tau}\right)_T = -(\rho^2/12)\, \xi_1 / \Sigma_\alpha\, \alpha^2\, \xi_\alpha \tag{139}$$

$$\bar{N} = \Sigma_\alpha\, \alpha\, \xi_\alpha / \Sigma_\alpha\, \xi_\alpha \tag{140a}$$

$$\left(\frac{\partial \bar{N}}{\partial \tau}\right)_T = \left[\alpha\left(\frac{d\xi_\alpha}{d\tau}\right)_T / \Sigma_\alpha\, \xi_\alpha\right] + \left[\left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T (-\rho/12)/(\Sigma_\alpha\, \xi_\alpha)^2\right] \quad (140b)$$

$$\left(\frac{\partial \bar{N}}{\partial T}\right)_\tau = \left[\alpha\left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau / \Sigma_\alpha\, \xi_\alpha\right] + \left[\left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau (-\rho/12)/(\Sigma_\alpha\, \xi_\alpha)^2\right] \quad (140c)$$

5.5. THERMODYNAMICS AND COMPOSITIONS ABOVE 7000° K

Reliable data for the free energies and enthalpies for the species C_α, $2 \le \alpha \le 10$, have not yet been calculated above 7000° K. However, at all densities of interest the system composition can be calculated at 7000° K. Further, we know that, at all densities of interest, at a sufficiently high temperature there will only be carbon atoms present. In order to bridge this gap, the following equations are assumed (in which we denote all quantities relevant to the point (τ, $T_o \equiv 7000°$ K) with the subscript "o" and all quantities at the upper limiting value with the subscript "u"):

$$\bar{N} = \bar{N}_o + (T - T_o)\left(\frac{\partial \bar{N}_o}{\partial T}\right)_\tau \quad (141)$$

$$\left(\frac{\partial \bar{N}}{\partial T}\right)_\tau = \left(\frac{\partial N_o}{\partial T}\right)_\tau \quad (142)$$

$$\bar{N}_u \equiv 1 \quad (143)$$

$$T_u = T_o - (\bar{N}_0 - \bar{N}_u)/\left(\frac{\partial \bar{N}_o}{\partial T}\right)_\tau \quad (144)$$

Thus, since T_o and $\bar{N}_u$ are constants,

$$(\partial T_u/\partial \tau)_T = -\left(\frac{\partial \bar{N}}{\partial \tau}\right)_T / (\partial \bar{N}_o/\partial T)_\tau \quad (145)$$

$$E = (\bar{N})^{-1}\, \bar{N}_o E_o + (T_o - T)(T_u - T_o)^{-1} \quad (146)$$

$$(\bar{N}_o E_o - E_u)$$

$$E_u = E_1(T_u) \quad (147)$$

$$\left(\frac{\partial E}{\partial T}\right)_\tau = \left|\left[-E\left(\frac{\partial \bar{N}}{\partial T}\right)_\tau - (T_u - T_o)^{-1}(\bar{N}_o E_o - E_1)\right]/\bar{N}\right| - \frac{3R}{2\bar{N}} \tag{148}$$

$$\left(\frac{\partial E}{\partial \tau}\right)_T = -\left(\frac{\partial \bar{N}}{\partial \tau}\right)_T \frac{E}{N} + (\bar{N})^{-1}\left|\left|\left(\frac{\partial \bar{N}_o}{\partial \tau}\right)_{T_o} E_o + \bar{N}_o\left(\frac{\partial E_o}{\partial \tau}\right)_T\right|\right| \left|1 + \frac{T_o - T}{T_u - T_o}\right| \frac{\left|\bar{N}E - \bar{N}_o E_o\right|}{(T_u - T_o)} \left(\frac{\partial T_u}{\partial \tau}\right)_T \tag{149}$$

To be consistent with the technique used above 7000° K, if $T > T_u$, we assume that

$$\xi_1 = \rho/12 \tag{150}$$

$$\left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T = \left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau = \left(\frac{\partial E_{sp}}{\partial \tau}\right)_T = 0 \tag{151}$$

$$\bar{N} = 1 \tag{152}$$

$$P = RT(\rho/12) \tag{153}$$

$$E_{sp} = E_1/12 \tag{154}$$

$$(\partial E_{sp}/\partial T)_\tau = \frac{dE_1}{dT}/12 \tag{155}$$

$$\left(\frac{\partial P}{\partial T}\right)_\tau = P/T \tag{156}$$

$$\left(\frac{\partial P}{\partial \tau}\right)_T = -P/\tau \tag{157}$$

5. 6. LOW TEMPERATURE RESULTS

Preliminary numerical calculations indicated that for $T < 1000^\circ K$, it is satisfactory to assume that

$$\xi_9 = \rho/108 \tag{158}$$

$$\bar{N} = 9 \tag{159}$$

$$\xi_{\alpha \neq 9} = 0 \tag{160}$$

$$\left(\frac{\partial P}{\partial T}\right)_\tau = P/T \tag{161}$$

$$\left(\frac{\partial E_{sp}}{\partial T}\right)_\tau = \frac{dE_9/dT}{108} \tag{162}$$

$$\left(\frac{\partial P}{\partial \tau}\right)_T = -P/\tau \tag{163}$$

$$P = \frac{RT}{108\tau} \tag{164}$$

$$E_{sp} = E_9/108 \tag{165}$$

$$\left(\frac{\partial \xi_\alpha}{\partial \tau}\right)_T = \left(\frac{\partial \xi_\alpha}{\partial T}\right)_\tau = \left(\frac{\partial E_{sp}}{\partial \tau}\right)_T = 0 \tag{166}$$

5. 7. COEFFICIENTS OF FITS TO THERMODYNAMIC FUNCTIONS

Table IV contains the $A_{\alpha,j}$, $\alpha = 1 \ldots 10$, $j = 1 \ldots 6$ used to fit

$$\left(\frac{G^\circ(T) - H^\circ(0)}{RT}\right)_\alpha = A_{\alpha,1}(1 - \ln T) - A_{\alpha,2} T - A_{\alpha,3}\frac{T^2}{2} - A_{\alpha,4}\frac{T^3}{3} - A_{\alpha,5}\frac{T^4}{4} - A_{\alpha,6} \tag{167}$$

Table IV

IDEAL GAS THERMODYNAMIC FUNCTIONS FOR C_α

C_α	$A_{\alpha,1}$	$A_{\alpha,2}$	$A_{\alpha,3}$	$A_{\alpha,4}$	$A_{\alpha,5}$	$A_{\alpha,o}$	$\Delta H^o(O)$ (cal/mole)	Range of Fit ($\times 10^3$ °K)
C	2.616739-00	-1.075931-04	3.860104-08	-4.508465-12	1.825810-16	4.114400-00	1.69580-05	0.3-6
C_2	4.608300-00	-4.309474-04	2.553405-07	-5.060553-11	3.488775-15	-1.851498-00	1.97000-05	0.3-o
C_3	4.061127-00	2.501656-03	-1.491669-06	5.338941-10	-7.682421-14	1.015292-00	1.88104-05	0.3-2
C_4	5.670072-00	2.941491-03	-1.583799-06	5.873590-10	-9.296338-14	-4.252196-00	2.40500-05	0.3-2
C_5	7.279097-00	3.381009-03	-1.675500-06	6.405815-10	-1.090542-13	-1.310398-01	2.40298-05	0.3-2
C_6	8.887801-00	3.821788-03	-1.768910-06	6.947653-10	-1.253361-13	-1.837056-01	2.87000-05	0.3-2
C_7	1.049661-01	4.262157-03	-1.861752-06	7.486224-10	-1.415519-13	-2.722151-01	2.87000-05	0.3-2
C_8	1.210560-01	4.701797-03	-1.953615-06	8.019347-10	-1.576603-13	-3.248919-01	3.39000-05	0.3-2
C_9	1.371412-01	5.143305-03	-2.048004-06	8.566633-10	-1.740497-13	-4.133905-01	3.34000-05	0.3-2
C_{10}	1.532298-01	5.583472-03	-2.140608-06	9.104058-10	-1.902459-12	-4.660623-01	3.93000-05	0.3-2
C_3	4.577017-00	1.135460-03	-2.083718-07	1.709699-11	-4.957820-16	-9.902669-01	1.88104-05	1.5-o
C_4	6.077354-00	1.721887-03	-3.159955-07	2.336921-11	-3.583350-16	-5.883521-00	2.40500-05	1.5-6
C_5	7.577380-00	2.308765-03	-4.238504-07	2.969125-11	-2.247249-16	-1.436729-01	2.40298-05	1.5-6
C_6	9.077268-00	2.895836-03	-5.318001-07	3.603287-11	-9.256675-17	-1.926238-01	2.87000-05	1.5-6
C_7	1.057812-01	3.481519-03	-6.390447-07	4.222393-11	5.109466-17	-2.774611-01	2.87000-05	1.5-6
C_8	1.207925-01	4.066801-03	-7.460864-07	4.837172-11	1.980545-16	-3.264719-01	3.39000-05	1.5-o
C_9	1.357901-01	4.654071-03	-8.541425-07	5.473711-11	3.283272-16	-4.112566-01	3.34000-05	1.5-6
C_{10}	1.507952-01	5.240247-03	-9.616407-07	6.098287-11	4.677693-16	-4.602377-01	3.93000-05	1.5-6

and

$$\left(\frac{H^o(T) - H^0(0)}{RT}\right)_\alpha = A_{\alpha,1} + A_{\alpha,2}T + A_{\alpha,3}T^2 + A_{\alpha,4}T^3 + A_{\alpha,5}T^4 \quad (168)$$

(The above equations are the same as Eqs. (118) and (119), respectively.)

5.8. INTERFACE OF CMOL WITH OTHER EQUATION OF STATE SUBROUTINES

In the SPUTTER code, the generalized ionic equation of state subroutines "EIONX"* are designed to interface with molecular equations of state in the following manner:

1. All ionization contributions are calculated by the EIONX routine
2. All translation contributions are calculated by the EIONX routine. If a molecular E. O. S. is not called by the EIONX routine, EIONX sets $\bar{N} = 1$, $(\partial\bar{N}/\partial\theta)_\tau = 0$, and $(\partial\bar{N}/\partial\tau)_\theta = 0$, where θ is the temperature in ev (see below) If a molecular E. O. S. is called, these quantities are calculated by that routine and returned to EIONX to be used.
3. The reference state for energy is assumed to contain only atoms.

The equations which have been presented have included the translational contributions, and the temperature scale has been in degrees Kelvin. The code actually uses a temperature scale in ev (1 ev $\cong$ 11605° K). The translational contributions to E and $(\partial E/\partial\theta)_\tau$ are subtracted before these quantities are passed on by CMOL to the EIONX code. This gives

$$E_{\text{EIONX input}} = E_{\text{CMOL}} - \frac{3}{2} RT\, C/\bar{N} - E_o \quad (169)$$

$$\left(\frac{\partial E}{\partial\theta}\right)_\tau, \text{ EIONX input} = \left(\frac{\partial E}{\partial\theta}\right)_\tau, \text{ CMOL} - C^1/\bar{N} \quad (170)$$

---

* See Section III of this report.

where C and C^1 are the appropriate conversion factors. The corresponding factor does not have to be subtracted out of P since only $\bar{N}$ is transferred to the EIONX code. The derivatives of P that are calculated and transferred to the EIONX code also exclude the translational contribution since they are calculated as

$$\left(\frac{\partial P}{\partial \theta}\right)_\tau = \left(\frac{\partial P}{\partial \bar{N}}\right)_{T,\tau} \left(\frac{\partial \bar{N}}{\partial T}\right)_\tau \left(\frac{\partial T}{\partial \theta}\right) \tag{171}$$

$$\left(\frac{\partial P}{\partial \tau}\right)_\theta = \left(\frac{\partial P}{\partial \bar{N}}\right)_{T,\tau} \left(\frac{\partial \bar{N}}{\partial \tau}\right)_T \tag{172}$$

5.9. FUTURE IMPROVEMENTS

Several of the assumptions will be replaced by a more extended treatment as soon as possible:

1. A program is under way to (a) compute high temperature partition functions, and (b) fit the resultant free energies and enthalpies in a thermodynamically consistent least-square manner. As soon as this is done, the "bridging" section will be removed from the code. This will be done initially for C_α, $1 \leq \alpha \leq 10$.
2. Following this, an attempt will be made to estimate the thermodynamic quantities for C_β, $11 \leq \beta \leq 20$. Calculations with the present system show that $\xi_9 >> \xi_{\alpha \neq 9}$ at $T \leq 1000°K$. However, this is only an artifice due to the exclusion of $C_{\beta>10}$ from the calculations. Inclusion of these species is expected to change the results at low temperatures so that $\bar{N} > 9$ at low temperatures.
3. An attempt will be made to add "real gas" correction factors for the various species.

5.10. VARIABLE NAMES USED IN CMOL

1.	A(10)	$A_{\alpha,1}$; $1 \le \alpha \le 10$ in Eq. (167) for $T \ge 1750°$ K.
2.	A2(10)	$A_{\alpha,1}$; $1 \le \alpha \le 10$ in Eq. (167); for $T < 1750°$ K.
3.	B(10)	$A_{\alpha,2}$; $1 \le \alpha \le 10$ in Eq. (167); for $T \ge 1750°$ K.
4.	B2(10)	$A_{\alpha,2}$; $1 \le \alpha \le 10$ in Eq. (167); for $T < 1750°$ K.
5.	BACK1	Previous Iterate.
6.	C(10)	$A_{\alpha,3}$; $1 \le \alpha \le 10$ in Eq. (167); $T \ge 1750°$ K.
7.	C2(10)	$A_{\alpha,3}$; $1 \le \alpha \le 10$ in Eq. (167); $T < 1750°$ K.
8.	CARBNZ(10)	Routine out put array; see section 5.9.
9.	COEF(11)	a^1_α; $1 \le \alpha \le 11$; see Eqs. (124c) and (124d).
10.	CONST	$a^1_{11} = -\rho/12$; see Eqs. (122e) and (124d).
11.	D(10)	$A_{\alpha,4}$; $1 \le \alpha \le 10$ in Eq. (167); $T \ge 1750°$ K.
12.	DZ(10)	$A_{\alpha,4}$; $1 \le \alpha \le 10$ in Eq. (167); $T < 1750°$ K.
13.	DCONDT	$\Sigma_\alpha \left(\partial \xi_\alpha / \partial T\right)_\tau$.
14.	DEDT(10)	$dE_\alpha/dT = R\left[A_{\alpha,1} - 1 + \Sigma_{j=2}^{j=5} \alpha A_{\alpha,j} T^j\right]$.
15.	DEDTAU	$(\partial E/\partial \tau)\theta$.
16.	DEDTHT	$(\partial E/\partial \theta)\tau$.
17.	DELH(10)	$H^o_\alpha(0)$.
18.	DNDT	$(\partial \bar{N}/\partial T)\tau$.
19.	DNDTAU	$(\partial \bar{N}/\partial \tau)T$.
20.	DPDN	$(\partial P/\partial \bar{N})T, \rho$.
21.	DPOTAU	$(\partial P/\partial \tau)\theta$.
22.	DPDTHT	$(\partial P/\partial \theta)\tau$.

23.	DREACT(10)	$-\alpha H_1^o(T)/RT - H_\alpha^o(T)/RT$.
24.	DXDT(10)	$(\partial\xi\alpha/\partial T)\tau$; $1 \le \alpha \le 10$.
25.	DXDTAU(10)	$(\partial\xi\alpha/\partial\tau)T$; $1 \le \alpha \le 10$.
26.	E(10)	$A_{\alpha,5}$; $1 \le \alpha \le 10$ in Eq. (167); $T < 1750°$ K.
27.	E2(10)	$A_{\alpha,5}$; $1 \le \alpha \le 10$ in Eq. (167); $T < 1750°$ K.
28.	EDIF	$E_o \bar{N}_o - E_1$.
29.	EION(20)	EIONX input - out put array; see Section III of this report.
30.	ENERGY	Specific energy in ergs/g; see Eq. (129).
31.	E0	$E_o = E(7000° K, \rho)$.
32.	E0NBAR	$E_o N_o$.
33.	ESPECZ(10)	$E_\alpha^o(T) = H_\alpha^o(T) - RT$.
34.	EI	$E(T_u)$.
35.	EZERO	Assumed specific energy of atomization (of graphite) ; 5.98566 E11 ergs/g.
36.	FK(10)	$A_{\alpha,6}$; $1 \le \alpha \le 10$ in Eq. (167); $T \ge 1750°$ K.
37.	FK2(10)	$A_{\alpha,6}$; $1 \le \alpha \le 10$ in Eq. (167); $T < 1750°$ K.
38.	FOFX	See Eq. (11e).
39.	FOFXM1	f (previous iterate); see Eq. (122e).
40.	FRENRG(10)	$\left[G_\alpha^o(T)\right]$ RT; $1 \le \alpha \le 10$.
41.	HSPECZ(10)	$H_\alpha^o(T)$.
42.	NBAR	Mean number of atoms per molecule; see Eq. (140a).
43.	NBAR0	$\bar{N}_o = \bar{N}(7000° K, \rho)$.

44.	PRESHR	P ; see Eq. (126).
45.	RTKEL	RT with R = 1.98726 cal/mole-° K.
46.	R2TKEL	RT with R = 82.06 cm^3/atm-° K.
47.	SUMCON	$\Sigma_\alpha \xi_\alpha$.
48.	SUMNRG	$\Sigma_\alpha \xi_\alpha E^o_\alpha (T)$.
49.	SUM1DX	$-\left\|\Sigma_\alpha \alpha \xi_\alpha \left[\alpha H^o_1 (T) + H^o_\alpha (T)\right]\right\| /RT$.
50.	SUM2DX	$\Sigma_\alpha \alpha^2 \xi_\alpha$.
51.	SUM3DX	$\Sigma_\alpha (\partial \xi_\alpha / \partial \tau)T$.
52.	SUM4DX	$\Sigma_\alpha (\partial \xi_\alpha / \partial \tau)T \left[E^o_\alpha (T)\right]$.
53.	SUM5DX	$\Sigma_\alpha (\partial \xi_\alpha / \partial T)\tau \left[E^o_\alpha (T)\right]$.
54.	SUM6DX	$\Sigma_\alpha \xi_\alpha (dE_\alpha / dT)$.
55.	SUM7DX	$\Sigma_\alpha \alpha (\partial \xi_\alpha / \partial T)\tau$.
56.	SUM8DX	$\Sigma_\alpha \alpha (\partial \xi_\alpha / d\tau)T$.
57.	T	Storage cell for T in computations above 7000° K.
58.	TAU	Specific volume in cm^3/g.
59.	TDGDT(10)	$-\left[H^o_\alpha (T)\right] /RT$.
60.	TDIF	T - 7000° K.
61.	TKEL	Temperature in ° K.
62.	TKELN	ln T.
63.	TUPM7	T_u - 7000° K.
64.	UPPERT	t_u ; see Eq. (144).
65.	X	$X = \xi_1 e^{G_1/RT} /RT$.
66.	XSET(10)	ξ_α ; $1 \leq \alpha \leq 10$.

67. XTRY — Regula falsi prediction of next iterate in Eq. (124a).

68. Y — Lower bound on X; $0 \leq Y$.

69. Z — Upper bound on X; $Z \leq (\rho/12)(RT)(e^{G_1/RT})$.

5.11. APPENDIX: LISTING OF CMOL

```
WIT FOR    MESTER/A,MESTER/A,MESTER/A1
      SUBROUTINE CMOL(X1, X2, X3)
C     ENERGY ZERO IS ATOMIZED CARBON (ENERGY=5.98566E11 ERGS/G.)
C              LAST COMPILED DECEMBER 12, 1965
C     X1 IS TAU IN G/CC
C     X2 IS THETA IN EV
C     X3 .LT. 0. FORCES TRANSLATIONAL-ONLY COMPUTATION
C     X3 .GT. 0. FORCES CUTOFF AT 1500. DEGREES KELVIN
C
      COMMON/LMS/EION(20)
      COMMON /LMSG/CARBNZ(10)
      REAL NBAR
      REAL NBARO
      EQUIVALENCE(OLDNRG,EION(15)),  (NBAR,EION(17))
      DIMENSION   A(10),B(10),C(10),D(10),E(10),FK(10),DELH(10),ERENRG(1
     10),ESPECZ(10),XSET(10),COEF(11)
      EQUIVALENCE(COEF(11),CONST)
      DIMENSION  HSPECZ(10),A2(10),B2(10),C2(10),D2(10),E2(10),FK2(10)
      DIMENSION TDGDT(10),DEDT(10),DXDT(10),DXDTAU(10),DREACT(10)
      DATA A/2.6167394,4.6083,4.5770171,6.0773536,7.57738,9.0772684,10.5
     178120,12.07925,13.579007,15.07952/
      DATA B/-1.0759307E-4,-4.3094741E-4,1.1354603E-3,1.7218871E-3,2.308
     17653E-3,2.8958363E-3,3.4815191E-3,4.0668009E-3,4.6540713E-3,5.2402
     2472E-3/
      DATA C/3.8601044E-8,2.5534049E-7,-2.0837176E-7,-3.1599548E-7,-4.23
     185044E-7,-5.3180008E-7,-6.3904472E-7,-7.4608642E-7,-8.5414254E-7,-
     29.6164066E-7/
      DATA D/-4.5084646E-12,-5.0605532E-11,1.7096995E-11,2.3369207E-11,2
     1.9691251E-11,3.6032875E-11,4.2223928E-11,4.8371722E-11,5.4737111E-
     211,6.0982872E-11/
      DATA E/1.8256099E-16,3.4887751E-15,-4.9578196E-16,-3.5P33503E-16,-
     12.2472492E-16,-9.2566753E-17,5.1094666E-17,1.9305455E-16,3.2832721
     2E-16,4.677695E-16/
      DATA FK/4.1144,-1.8514979,-.99026691,-5.8835212,-14.367287,-19.262
     1383,-27.746115,-32.647187,-41.125658,-46.023767/
      DATA DELH/1.6958E5,1.97E5,1.88104E5,2.405E5,2.40298E5,2.87E5,2.87E
     15,3.39E5,3.34E5,3.93E5/
C
C
      DATA A2/2.6167394,4.6083,4.0611273,5.6700722,7.2790966,8.8871007,1
     10.496602,12.105599,13.714116,15.322981/
      DATA B2/-1.0759307E-4,-4.3094741E-4,2.5016562E-3,2.9414906E-3,3.38
     110092E-3,3.8217876E-3,
     2          4.2621570E-3,4.7017969E-3,5.1433051E-3,5.5834718E-3/
      DATA C2/3.8601044E-8,2.5534049E-7,-1.491669E-6,-1.5837991E-6,
     1-1.6755E-6,-1.7689104E-6,
     2          -1.8617521E-6,-1.9536149E-6,-2.0480045E-6,-2.1406085E-6/
      DATA D2/-4.5084646E-12,-5.0605532E-11,5.3389410E-10,5.8735896E-10,
     16.4056152E-10,6.9476531E-10,7.4862238E-10,8.0193467E-10,8.566632RE
     2-10,9.1040577E-10/
      DATA E2/1.8258099E-16,3.4887751E-15,-7.6824207E-14,-9.296338UE-14,
     1-1.0905419E-13,-1.2533614E-13,-1.4155192E-13,-1.5766034E-13,-1.740
     24966E-13,-1.9024594E-13/
      DATA FK2/4.1144,-1.8514979,1.0152922,-4.2521956,-13.103985,-18.370
     156,-27.221515,-32.489186,-41.339045,-46.606231/
C
C
      EQUIVALENCE                    (PRESHR,CARBNZ(2)),(DEDTAU,CARBNZ(3)),
```

```
     1(DEDTHT,CARBNZ(4)),(DPDTAU,CARBNZ(5)),(DPDTHT,CARBNZ(6)),
     2(ENERGY,CARBNZ(1))
C
      TAU=        X1
      EZERO=      5.98566E11
         IF(X3 .LT. 0. .AND. A(1) .NE.2.5) GO TO 10
   11 CONTINUE
      IF( TAU.LT.1.E-1) GO TO 900
      T=          -1.
      UPPERT=     0.
      CONST=      -1./(12.*TAU)
      TKEL=       11605.4 * X2
         IF(TKEL.GT.7.E3) GO TO 550
  551 CONTINUE
C
      TKELN=      ALOG(TKEL)
      RTKEL=     1.98726*TKEL
      R2TKEL=     82.06*TKEL
C     1.98726 IS THE GAS CONSTANT IN CALORIES/MOLE/DEGREE KELVIN
C     82.06 IS THE GAS CONSTANT IN CC.-ATMOSPHERES/MOLE/DEGREE KELVIN
      DO 201 I=1,10
      IF (TKEL.LT.1750.) GO TO 400
      FRENRG(I)= A(I)*(1.- TKELN )   -(FK(I)+TKEL*(B(I)+TKEL*(C(I)/2.+
     1             TKEL*(D(I)/3.+TKEL*E(I)/4. ))))  +DELH(I)/RTKEL
      DEDT(I)=   1.98726*( A (I)-1.+TKEL*(2.*B (I)+TKEL*(3.*C(I)+TKEL*
     1             (4.*D(I)+TKEL*5.*E (I) ))))
  401 CONTINUE
      FI=         1
      COEF(I)=   FI*EXP(-FRENRG(I) )/R2TKEL
  201 CONTINUE
         IF(TKEL.LT.1.E3) GO TO 650
         IF(X3 .GT. 0. .AND. TKEL .LT. 1.5E3) GO TO 650
C
C     THE LOWER BOUND ON X IS 0.
      Y=          0.
C     DEVELOP UPPER BOUND TO X
      Z=          -CONST/COEF(1)
      IF ( Z.LE. 1.) GO TO 604
  602 CONTINUE
      DO 221 I=1,9
      J=          10-I
         IF(COEF(J).NE.0.) GO TO 222
  221 CONTINUE
  222 CONTINUE
         IF(COEF(1).EQ.0.) CALL UNCLE
      Z=          1.+((-CONST/COEF(J))**(1./FLOAT(J)))
      IF ( Z.LT. 2.) Z=  Z-1.
  604 CONTINUE
      X=          Z
      BACK1=      0.
      XTRY=      -1.E-38
      F OF XM1=0.
  211 CONTINUE
      DO 203 J= 1,25
      F OF X =   COEF(10)
      DO 204 I=1,9
      III=        10-I
```

```
      F OF )        F OF X *X + COEF(III)
  204 CONTINUE
      F OF X =      F OF X * X + CONST
      FJ=           J
      IF (F OF X .GT. 0.) Z= X
      IF (F OF X .LT. 0.) Y= X
      IF(J.EQ.1.AND.FOFX.GT.( -2.* CONST )) GO TO 212
      IF ( ABS(F OF X) .LT. (1.E- 6*(- CONST  )) ) GO TO 205
         IF (ABS(FOFX).GE.(-.1*CONST)) GO TO 206
      IF ( FOFX.EQ.FOFXM1) GO TO 206
  209 CONTINUE
      IF(J.GT.1) XTRY =  X - (X-BACK1)/(FOFX-FOFXM1)*F OF X
  206 CONTINUE
      BACK1=        X
      X=            (Z+Y)*.5
      IF ( F OF X .EQ. FOFXM1 ) GO TO 208
      IF (XTRY.GE.Y.AND.XTRY.LE.Z.AND.ABS(FOFX).LT.(-.1*CONST)) X=XTRY
  208 CONTINUE
      FOFXM1=F OF X
  203 CONTINUE
      J=            J-1
  297 CONTINUE
      CARBNZ(8)= 97.0297
      RETURN
  205 CONTINUE
      FJ=           J
C     PRESSURE
      SUMCON=       0.
      DO 301 I=1,10
      XSET(I)=      0.
         IF (COEF(I).EQ.0.) GO TO 301
      FI=           I
      XSET(I)= (COEF(I)/FI*X** (FI/2.))*X**(FI/2.)
      SUMCON=       SUMCON + XSET(I)
  301 CONTINUE
      NBAR=         -CONST   /SUMCON
      PRESHR=       1.01325E6*R2TKEL*SUMCON
C     ENERGY
      INITAL=       1
      LAST=         10
    4 CONTINUE
      SUMNRG=       0.
      DO 302 I=INITAL,LAST
      IF (TKEL.LT.1750.)GO TO 402
      HSPECZ(I)= RTKEL*(A(I)+TKEL*(B(I)+TKEL*(C(I)+TKEL*(D(I)+TKEL*E(I)
     1              ))))+DELH(I)
  403 CONTINUE
      ESPECZ(I)= HSPECZ(I) - RTKEL
      SUMNRG=       SUMNRG + XSET(I)*ESPECZ(I)
  302 CONTINUE
      ENERGY=       TAU*SUMNRG*4.185E7
         IF(TKEL.LT.1.E3) GO TO 601
      SUM1DX=       0.
      SUM2DX=       0.
      DO 500 I=1,10
      FI=           I
      TDGDT(I)=  -HSPECZ(I)/RTKEL
```

```
      DREACT(I)= FI*TDGDT(1)-TDGDT(I)
      SUM1DX=    SUM1DX+XSET(I)*FI*DREACT(I)
      SUM2DX=    SUM2DX + FI*FI*XSET(I)
  500 CONTINUE
      DXDT(1)=   -XSET(1)*(( CONST  +SUM1DX)/SUM2DX+1.)/TKEL
      DXDTAU(1)= -XSET(1)/(12.*TAU*TAU*SUM2DX)
      DO 501 I=2,10
      FI=I
      DXDT(1)=   XSET(I)*(FI/XSET(1)*DXDT(1)+(DREACT(I)+FI-1.)/TKEL)
      DXDTAU(I)= FI*DXDTAU(1)/XSET(1)*XSET(I)
  501 CONTINUE
      DCONDT=    0.
      SUM3DX=    0.
      SUM4DX=    0.
      SUM5DX=    0.
      SUM6DX=    0.
      SUM7DX=    0.
      SUM8DX=    0.
      DO 502 I=1,10
      FI=I
      DCONDT=    DCONDT + DXDT(I)
      SUM3DX=    SUM3DX+DXDTAU(I)
      SUM4DX=    SUM4DX+DXDTAU(I)*ESPECZ(I)
      SUM5DX=    SUM5DX+ESPECZ(I)*DXDT(I)
      SUM6DX=    SUM6DX+DEDT(I)*XSET(I)
      SUM7DX=    SUM7DX+FI*DXDT(I)
      SUM8DX=    SUM8DX+FI*DXDTAU(I)
  502 CONTINUE
      DNDT=      SUM7DX/SUMCON+DCONDT* CONST  /SUMCON/SUMCON
      DNDTAU=    SUM8DX/SUMCON+SUM3DX* CONST  /SUMCON/SUMCON
      DPDN=      -PRESHR/NBAR
      DPDTAU=    DPDN * DNDTAU
      DPDTHT=    DPDN * DNDT * 11605.4
      DEDTAU=    4.185E7*TAU*(SUM4DX+SUMNRG*SUM8DX/CONST)
      DEDTHT=    4.85686E11*TAU*(SUM5DX+SUM6DX+SUMNRG*SUM7DX/COEF(11))
         IF(T.NE.(-1.)) GO TO 503
      GO TO 901
  650 CONTINUE
      PRESHR=    -1.125833E5*R2TKEL*CONST
      INITAL=    9
      LAST=      9
      NBAR=      9.
      XSET(9)=   -CONST/9.
      GO TO 4
  601 CONTINUE
      DPDTAU=    0.
      DPDTHT=    0.
      DEDTAU=    0.
      DEDTHT=    4.4971E9*DEDT(9)
      GO TO 901
  212 CONTINUE
      X=         .1*X
      GO TO 211
  400 CONTINUE
      FRENRG(I)= A2(I)*(1.-TKELN)-(FK2(I)+TKEL*(B2(I)+TKEL*(C2(I)*.5+TKE
     1            L*(D2(I)/3.+TKEL*E2(I)*.25))))+DELH(I)/RTKEL
      DEDT(I)=   1.98726*( A2(I)-1.+TKEL*(2.*B2(I)+TKEL*(3.*C2(I)+TKEL*
```

```
     1              (4.*D2(I)+TKEL*5.*E2(I) ))))
      GO TO 401
  402 RSPEC2(I)= RTKEL*(A2(I)+TKEL*(B2(I)+TKEL*(C2(I)+TKEL*(D2(I)+TKEL*E
     1              2(I) )))) +DELH(I)
      GO TO 403
  550 CONTINUE
      T=          TKEL
         IF (T.GE.6.5E3 .AND. TAU.GE.1.E3 ) GO TO 504
         IF (T.GT.1.05E4 .AND. TAU.GE. 1. ) GO TO 504
         IF ( T .GE. 1.3E4 ) GO TO 504
      TKEL=       7.E3
      GO TO 551
C
  503 CONTINUE
      NBARO=      NBAR
      UPPERT=     7.E3-(NBARO-1.)/DNDT
         IF(T.GT.UPPERT) GO TO 504
      TUPM7=      UPPERT-7.E3
      TDIF=       T-7.E3
      NBAR=       NBAR+TDIF*DNDT
      EO=         ENERGY
      E1=         1.0392445E7*UPPERT+5.98566E11
      EONBAR=     EO*NBARO
      EDIF=       EONBAR-E1
      ENERGY=     (EONBAR-TDIF/TUPM7*EDIF)/NBAR
      DEDTHT=     -11605.4*(ENERGY*DNDT+EDIF/TUPM7)/NBAR
      DEDTAU=     (-ENERGY*DNDTAU +((UPPERT-T)/TUPM7)*(EO*DNDTAU+NBARO*
     1              DEDTAU) - EDIF/TUPM7 * DNDTAU/DNDT * TDIF/TUPM7)/NBAR
      PRESHR=    - CONST  /NBAR*T*8.3139564E7
      DPDTAU=     -PRESHR/NBAR*DNDTAU
      DPDTHT=     -PRESHR*11605.4*DNDT/NBAR
      TKEL=       T
  901 CONTINUE
      ENERGY=     ENERGY-1.0392445E7*TKEL/NBAR- EZERO
      DEDTHT=     DEDTHT-1.2060840E11/NBAR
  902 CONTINUE
      CARBN2(8)= 0.
      CARBN2(7)= NBAR
      RETURN
  504 CONTINUE
      ENERGY=     5.98566E11 - EZERO
      TKEL=       T
      PRESHR=     -  CONST *TKEL*8.3139564E7
      DPDTAU=     0.
      DPDTHT=     0.
      DEDTAU=0.
      DEDTHT=     0.
      NBAR=       1.
      XSET(1)=    -CONST
      GO TO 902
  900 CONTINUE
  197 CONTINUE
      CARBN2(8)= 97.0197
      RETURN
   10 CONTINUE
      DO 15 I=1,10
      A(1) = 2.5
```

```
      B(I) = 0.
      C(I) = 0.
      D(I) = 0.
      E(I) = 0.
      FK(I)= 0.
      A2(I)= 2.5
      B2(I)= 0.
      C2(I)= 0.
      D2(I)= 0.
      E2(I)= 0.
      FK2(I)=0.
   15 CONTINUE
      GO TO 11
      END
```

REFERENCE

1. Duff, Russell E., and S. H. Bauer, "Equilibrium Composition of the C/H System at Elevated Temperatures," J. Chem. Phys. 36, 1754 (1962).

Unclassified

Security Classification

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) General Atomic Division General Dynamics Corporation San Diego, California	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b. GROUP

3. REPORT TITLE

NUCLEAR EXPLOSION INTERACTION STUDIES
VOLUME II: METHODS FOR ANALYSIS OF THERMAL PHENOMENA

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

Final Report 22 July 1965 to 21 July 1966

5. AUTHOR(S) (Last name, first name, initial)

Pyatt, K. D., Jr., et al.

6. REPORT DATE May 1967	7a. TOTAL NO. OF PAGES 196	7b. NO. OF REFS 4
8a. CONTRACT OR GRANT NO. AF29(601)-7035 b. PROJECT NO. 5710 c. Subtask No. 07.002 d.	9a. ORIGINATOR'S REPORT NUMBER(S) AFWL-TR-66-108, Vol. II 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) Contractor's Report No. GA-7370	

10. AVAILABILITY/LIMITATION NOTICES This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of AFWL (WLRT), Kirtland AFB, N.M. Distribution of this document is limited because of the technology discussed.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Air Force Weapons Laboratory (WLRT) Kirtland Air Force Base, New Mexico 87117

13. ABSTRACT

Various analytic and numerical methods are described for the phenomena which take place when a high-energy-density source interacts with matter. The interaction usually begins with the transient heating of a solid surface for which analytical methods of study have been developed (Section I). The second phase of the interaction process is vaporization. Recent developments in numerical techniques for simulating vaporization are discussed in the context of the two-dimensional interaction code HECTIC (Section II). The third phase normally involves the nonsteady flow of ionized vapor, for which equations of state are required. A general numerical technique (EIONX) for evaluating internal energy and pressure for a given temperature and density has been developed and incorporated in the SPUTTER program (Section III). For computer programs, e.g., HECTIC, which use internal energy and density as the independent variables, numerical methods were developed to invert the equations of state generated by EIONX (Section IV). For relatively low energy-density sources, the vapor may be in a molecular phase for a significant part of the interaction process, thus requiring the development of special techniques for evaluating the molecular dissociation energy as a function of temperature and density. The calculations for one particular material--carbon--are discussed in detail (Section V).

(Distribution Limitation Statement No. 2)

DD FORM 1 JAN 64 1473

Unclassified

Security Classification

Unclassified
Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Heat conduction Vaporization Equations of state for ionized vapor Table look-up method						

INSTRUCTIONS

1. ORIGINATING ACTIVITY: Enter the name end eddress of the contractor, subcontractor, grentee, Department of Defense activity or other organizetion (*corporate author*) issuing the report.

2a. REPORT SECURITY CLASSIFICATION: Enter the overall security classification of the report. Indicate whether "Restricted Data" is included. Marking is to be in accordance with appropriate security regulations.

2b. GROUP: Automatic downgrading is specified in DoD Directive 5200.10 and Armed Forces Industrial Manuel. Enter the group number. Also, when applicable, show that optionel markings have been used for Group 3 and Group 4 as authorized.

3. REPORT TITLE: Enter the complete report title in all capital letters. Titles in all cases should be unclassified. If a meaningful title cannot be selected without classification, show title classificetion in all capitals in parenthesis immediately following the title.

4. DESCRIPTIVE NOTES: If appropriate, enter the type of report, e.g., interim, progress, summery, annual, or final. Give the inclusive dates when a specific reporting period is covered.

5. AUTHOR(S): Enter the name(s) of author(s) as shown on or in the report. Enter last name, first name, middle initial. If military, show rank and brench of service. The name of the principal author is an absolute minimum requirement.

6. REPORT DATE: Enter the dete of the report as day, month, year, or month, year. If more than one date appears on the report, use date of publicetion.

7a. TOTAL NUMBER OF PAGES: The total pege count should follow normel pegination procedures, i.e., enter the number of pages containing informetion.

7b. NUMBER OF REFERENCES: Enter the totel number of references cited in the report.

8a. CONTRACT OR GRANT NUMBER: If appropriate, enter the applicable number of the contract or grant under which the report wes written.

8b, 8c, & 8d. PROJECT NUMBER: Enter the eppropriate military department identificetion, such es project number, subproject number, system numbers, task number, etc.

9a. ORIGINATOR'S REPORT NUMBER(S): Enter the official report number by which the document will be identified and controlled by the originating activity. This number must be unique to this report.

9b. OTHER REPORT NUMBER(S): If the report has been assigned any other report numbers (*either by the originator* or *by the sponsor*), also enter this number(s).

10. AVAILABILITY/LIMITATION NOTICES: Enter any limitations on further disseminetion of the report, other than those imposed by security classificetion, using standard statements such as:

(1) "Qualified requesters may obtain copies of this report from DDC."

(2) "Foreign announcement and dissemination of this report by DDC is not authorized."

(3) "U. S. Government agencies may obtain copies of this report directly from DDC. Other quelified DDC users shall request through

_____."

(4) "U. S. military agencies mey obtain copies of this report directly from DDC. Other qualified users shall request through

_____."

(5) "All distribution of this report is controlled. Qualified DDC users shall request through

_____."

If the report has been furnished to the Office of Technical Services, Department of Commerce, for sale to the public, indicete this fact and enter the price, if known.

11. SUPPLEMENTARY NOTES: Use for additional explenatory notes.

12. SPONSORING MILITARY ACTIVITY: Enter the name of the departmental project office or leboretory sponsoring (*paying for*) the research end development. Include eddress.

13. ABSTRACT: Enter en abstract giving e brief and fectual summary of the document indicetive of the report, even though it mey also eppeer elsewhere in the body of the technical report. If edditional space is required, a continuation sheet shall be attached.

It is highly desirable that the abstract of classified reports be unclassified. Each paragraph of the abstract shall end with en indicetion of the military security classification of the informetion in the peregraph, represented as *(TS)*, *(S)*, *(C)*, or *(U)*.

There is no limitation on the length of the abstract. However, the suggested length is from 150 to 225 words.

14. KEY WORDS: Key words are technically meaningful terms or short phreses that characterize e report and mey be used as index entries for cataloging the report. Key words must be selected so that no security classificetion is required. Identifiers, such es equipment model designation, trade name, military project code name, geographic locetion, may be used as key words but will be followed by an indication of technical context. The assignment of links, rules, and weights is optional